

Bose crystal as a standing sound wave

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A new class of solutions for Bose crystals with a simple cubic lattice consisting of N atoms is found. The wave function (WF) of the ground state takes the form $\Psi_0 = e^{S_w^{(1)} + S_b} \prod_j \{\sin(k_{l_x} x_j) \sin(k_{l_y} y_j) \sin(k_{l_z} z_j)\}$, where e^{S_b} is the ground-state WF of a fluid, $S_w^{(1)} = \sum_{\mathbf{q} \neq 0} S_1^{(1)}(\mathbf{q}) \rho_{-\mathbf{q}} + \sum_{\mathbf{q}, \mathbf{k} \neq 0}^{\mathbf{q} + \mathbf{k} \neq 0} S_2^{(1)}(\mathbf{q}, \mathbf{k}) \rho_{\mathbf{k}} \rho_{-\mathbf{k} - \mathbf{q}} + \dots$, $\rho_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_{j=1}^N e^{-i\mathbf{k}\mathbf{r}_j}$, and $\mathbf{k}_l = (\pi/a_l, \pi/a_l, \pi/a_l)$ (a_l is the lattice constant). The state with a single longitudinal acoustic phonon is described by the WF $\Psi_{\mathbf{k}} = \left[\rho_{-\mathbf{k}} + \sum_{\mathbf{q}} P_2(\mathbf{k}, \mathbf{q}) N^{-1/2} \rho_{\mathbf{q}} \rho_{-\mathbf{k} - \mathbf{q}} + \sum_{q_x} Q_1(q_x) \rho_{-\mathbf{k} - \mathbf{q}_x} + 7 \text{ permutations} \right] \Psi_0$, where the permutations give the terms with different signs of components of \mathbf{k} . The structure of $\Psi_{\mathbf{k}}$ is such that the excitation corresponds, in fact, to the replacement of \mathbf{k}_l in some triple of sines from Ψ_0 by \mathbf{k} . Such a structure of Ψ_0 and $\Psi_{\mathbf{k}}$ means that the crystal is created by sound: the ground state of a cubic crystal is formed by N identical three-dimensional standing waves similar to a longitudinal sound. It is also shown that the crystal in the ground state has a condensate of atoms with $\mathbf{k} = \mathbf{k}_l$. The nonclassical inertia moment observed in crystals He^4 can be related to the synchronous tunneling of condensate atoms.

PACS numbers: 61.50.Ah, 67.80.-s, 67.80.bd, 67.80.de

I. INTRODUCTION

The science on crystals is developed for many years, and most properties of crystals are successfully explained. The current interest is focused on the regions of unconventional and yet unguessed properties manifesting themselves, in particular, at extra-low temperatures (see surveys¹⁻³). For the crystals with a charged lattice and the Bose crystals, such regions are, respectively, high-temperature superconductivity and supersolid phenomena. The splash-up of interest arose after the excellent experiments by E. Kim and M. Chan^{4,5}, where a nonclassical inertia moment (NCIM) of a crystal He^4 was discovered. Later on, a number of new interesting properties joined by the term “supersolid” were found⁶⁻¹⁶. There are almost no doubts that the “supersolid” phenomenon is related to the superfluidity of quantum crystals, which was predicted long ago¹⁷. However, the physical nature of the superfluidity and the “supersolid” phenomenon is not clear yet, though a lot of models were developed¹⁸⁻²⁸.

The results obtained below indicate that the basic property of crystals, i.e., the nature of crystalline ordering, is not completely clear as well.

Commonly accepted is the following structure of the WF of a Bose crystal²⁹⁻³²:

$$\Psi_0 = e^{-\sum_{i>j} S_J(\mathbf{r}_i - \mathbf{r}_j)} \prod_{i=1}^N \varphi(\mathbf{r}_i - \mathbf{R}_i), \quad (1)$$

where N is the total number of atoms of a crystal, \mathbf{r}_j and \mathbf{R}_j are coordinates of atoms and sites of the lattice, the exponential function is the Bijl-Jastrow function taking correlations into account, and $\varphi(\mathbf{r})$ is usually written in the approximation of small oscillations: $\varphi(\mathbf{r}) = e^{-\alpha^2 r^2/2}$.

By the modern ideas, a crystal is formed since its energy is less than that of a fluid.

In what follows, we propose the basically new wave solution for the WF of a Bose crystal. In Ref. 33 (cited below as I), it was shown that the states of a system of N interacting Bose particles positioned in a rectangular box $L_x \times L_y \times L_z$ in size include the states with the WF

$$\Psi_0 = A e^{S_w^{(1)} + \tilde{S}_b} \prod_{j=1}^N \{\sin(k_{l_x} x_j) \sin(k_{l_y} y_j) \sin(k_{l_z} z_j)\}, \quad (2)$$

where $(k_{l_x}, k_{l_y}, k_{l_z}) \equiv \mathbf{k}_l = (l_x \pi/L_x, l_y \pi/L_y, l_z \pi/L_z)$, l_x, l_y, l_z are integers, and the remaining designations are given in Sec. 2. In I, we analyzed Ψ_0 only with $\mathbf{k}_l = \mathbf{k}_1 = (\pi/L_x, \pi/L_y, \pi/L_z)$ (here, $l_x, l_y, l_z = 1$), which describes the ground state of a gas and a fluid. In this case, the sines in (2) form a standing half-wave that covers the whole system and rests on the boundaries. But, l_x, l_y and l_z may obviously take in the solution any other integer values except zero. It is natural to assume that if the half-wave is equal to the lattice constant, then WF (2) describes a rectangular crystal lattice. Moreover, (2) is one of the exact solutions of the Schrödinger equation with zero boundary conditions (BCs). In what follows, we will study this solution and the solution for a longitudinal acoustic phonon. We will show that the solutions agree with observable properties of crystals and predict a number of specific features, in particular, the condensates of phonons and atoms in a crystal. Solution (2) testifies to the *wave nature of a crystal*. I did not deal with crystals earlier and have found the solutions accidentally, while studying the microstructure of a fluid.

A short announcement of the results will be published separately³⁴.

II. GROUND STATE OF A CRYSTAL

Due to the presence of a product of sines in Ψ_0 (2), the system can be partitioned into $l_x \times l_y \times l_z$ identical domains separated by plane surfaces, on which $\Psi_0 = 0$. We may assume that if each domain contains one atom, and the size of domains is close to the equilibrium interatomic distance, then the system is stable. A crystal corresponds, obviously, to a system of domains with the size at which the energy of the system is minimum. If the number of domains is equal to the number of atoms, then $l_x = L_x/\bar{R}_x$, $l_y = L_y/\bar{R}_y$, $l_z = L_z/\bar{R}_z$, where \bar{R}_x , \bar{R}_y and \bar{R}_z are the periods of the lattice along the appropriate axes. For a cubic crystal, they are equal to \bar{R} . Let us study the properties of such system and make clear whether they correspond to the properties of crystals. We consider only a simple cubic (sc) lattice.

Consider WF (2). In it, \tilde{S}_b is given by the formula (see I)

$$\begin{aligned} \tilde{S}_b = & \sum_{\mathbf{k}_1 \neq 0}^{(\pi)} \frac{a_2(\mathbf{k}_1)}{2!} \rho_{\mathbf{k}_1} \rho_{-\mathbf{k}_1} \\ & + \sum_{\mathbf{k}_1, \mathbf{k}_2 \neq 0}^{(\pi) \mathbf{k}_1 + \mathbf{k}_2 \neq 0} \frac{a_3(\mathbf{k}_1, \mathbf{k}_2)}{3! \sqrt{N}} \rho_{\mathbf{k}_1} \rho_{\mathbf{k}_2} \rho_{-\mathbf{k}_1 - \mathbf{k}_2} + \dots, \end{aligned} \quad (3)$$

where

$$\rho_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_{j=1}^N e^{-i\mathbf{k}\mathbf{r}_j} \quad (\mathbf{k} \neq 0), \quad (4)$$

and the summation is carried on over the wave vectors

$$\mathbf{k} = \pi \left(\frac{j_x}{L_x}, \frac{j_y}{L_y}, \frac{j_z}{L_z} \right) \quad (5)$$

(j_x, j_y, j_z are integers), which are multiple to π/L . This is denoted by the symbol (π) above the sums (under cyclic BCs, \mathbf{k} are multiple to $2\pi/L$, and the solutions are strongly changed). The function $S_w^{(1)}$ in (2) takes the form of an infinite series (see I)

$$\begin{aligned} S_w^{(1)} = & \sum_{\mathbf{q} \neq 0} S_1^{(1)}(\mathbf{q}) \rho_{-\mathbf{q}} + \sum_{\mathbf{q}, \mathbf{k}_1 \neq 0}^{\mathbf{q} + \mathbf{k}_1 \neq 0} \frac{S_2^{(1)}(\mathbf{q}, \mathbf{k}_1)}{\sqrt{N}} \rho_{\mathbf{k}_1} \rho_{-\mathbf{k}_1 - \mathbf{q}} + \\ & + \sum_{\mathbf{q}, \mathbf{k}_1, \mathbf{k}_2 \neq 0}^{\mathbf{q} + \mathbf{k}_1 + \mathbf{k}_2 \neq 0} \frac{S_3^{(1)}(\mathbf{q}, \mathbf{k}_1, \mathbf{k}_2)}{N} \rho_{\mathbf{k}_1} \rho_{\mathbf{k}_2} \rho_{-\mathbf{k}_1 - \mathbf{k}_2 - \mathbf{q}} + \dots \end{aligned} \quad (6)$$

where \mathbf{k}_j run values (5), and \mathbf{q} take values $2\pi \left(\frac{j_x}{L_x}, \frac{j_y}{L_y}, \frac{j_z}{L_z} \right)$. In (3), the first sum is the Bijl-Jastrow function written in the variables $\rho_{\mathbf{k}}$.

Let the faces of the crystal be ideally plane and parallel to atomic planes of the lattice. Every face creates a potential barrier for atoms of the crystal. We model this barrier for the face that is perpendicular to the X and

has the coordinate $x = 0$ by a step

$$U_w(x) \approx \begin{cases} U_s & x \leq 0, \\ 0 & x > 0. \end{cases} \quad (7)$$

The potential of the face with the coordinate $x = L_x$ is $U_w(L_x - x)$. Analogously, we can consider four other faces. For simplicity, we take $U_w = \infty$, which corresponds to zero BCs.

In I, the product of assigning sines

$$\Psi_{sc}^{bare}(N) = \prod_{j=1}^N \{ \sin(k_{l_x} x_j) \sin(k_{l_y} y_j) \sin(k_{l_z} z_j) \} \quad (8)$$

has been factor out from the equations for Ψ_0 and $\Psi_{\mathbf{k}}$. In this case, we obtain the cotangent $\cot(\pi l_x x / L_x)$, which cannot be expanded in a Fourier series, because $\int_0^{L_x} |\cot(\pi l_x x / L_x)| dx = \infty$. To overcome this problem, we will use the following. It is easy to see that, under the change $\sin kx \rightarrow |\sin kx|$, the derivative $(d|\sin kx|/dx)(1/|\sin kx|)$ gives again $\cot(kx)$. Therefore, we replace Ψ_{sc}^{bare} (8) by the WF

$$\Psi_{sc}^{bare}(N) = \prod_{j=1}^N \{ |\sin(k_{l_x} x_j)| \times |\sin(k_{l_y} y_j)| \times |\sin(k_{l_z} z_j)| \} \quad (9)$$

and pass to

$$\begin{aligned} \Psi_{sc}^{bare}(N) = & \prod_{j=1}^N \{ (|\sin(k_{l_x} x_j)| + \delta) \\ & \times (|\sin(k_{l_y} y_j)| + \delta) \times (|\sin(k_{l_z} z_j)| + \delta) \}, \end{aligned} \quad (10)$$

where $\delta > 0, \delta \rightarrow 0$. For such Ψ_{sc}^{bare} , we obtain the function

$$\tilde{f}(x) = (df/dx)(1/f), \quad f = |\sin(k_{l_x} x)| + \delta \quad (11)$$

instead of $\cot(k_{l_x} x)$. The former can be expanded in a Fourier series. For the singular point x_0 , the series gives the arithmetic mean value of those at the points $x_0 - 0$ and $x_0 + 0$. In the final formulas, we transit to the limit $\delta \rightarrow 0$, which returns us to functions (9) and (8). Bearing this fact in mind, we will immediately use in formulas the expansions at $\delta = 0$:

$$\cot(k_{l_x} x) \equiv \cot(\pi l_x x / L_x) = \sum_{j_x} C_{l_x}(q_x) e^{iq_x x}. \quad (12)$$

Here, $q_x = 2\pi j_x / L_x$, j_x runs all integers, and

$$C_{l_x}(q_x) \equiv C_{l_x}(j_x) = \begin{cases} -i & \text{for } j_x = l_x, 2l_x, 3l_x, \dots \\ i & \text{for } j_x = -l_x, -2l_x, -3l_x, \dots \\ 0 & \text{for the rest } j_x. \end{cases} \quad (13)$$

The proof of formulas (12) and (13) is given in Appendix.

We now have all the required in order to write the WFs of a Bose crystal. The WF of the ground state

is set by formula (2), where \tilde{S}_b and $S_w^{(l)}$ are given by formulas (3) and (6). The equations for the functions a_l and the ground-state energy of an atom (E_0) follow from equations in I with the changes $\mathbf{k}_1 \rightarrow \mathbf{k}_l \equiv \mathbf{k}_c$, $C_1(q) \rightarrow C_l(q)$, $S_j^{(1)} \rightarrow S_j^{(l)}$:

$$E_0 = \tilde{E}_0^b + A_1, \quad (14)$$

$$A_1 = \frac{\hbar^2}{2m} \left[k_c^2 - \frac{1}{N} \sum_{\mathbf{q} \neq 0}^{(2\pi)} q^2 S_1^{(l)}(\mathbf{q}) S_1^{(l)}(-\mathbf{q}) \right. \\ \left. - \frac{i}{\sqrt{N}} \sum_{q_x \neq 0}^{(2\pi)} 2k_{cx} q_x C_{l_x}(q_x) S_1^{(l)}(-\mathbf{q}_x) + (x \rightarrow y, z) \right], \quad (15)$$

$$\tilde{E}_0^b = \frac{N-1}{2^{d+1}N} n\nu_3(0) - \frac{1}{2^{d+1}N} \sum_{\mathbf{k} \neq 0}^{(\pi)} n\nu_3(k) - \frac{1}{N} \sum_{\mathbf{k} \neq 0}^{(\pi)} \frac{\hbar^2 k^2}{2m} a_2(\mathbf{k}), \quad (16)$$

$$\frac{n\nu_3(k)m}{2^d \hbar^2} + a_2(\mathbf{k})k^2 - a_2^2(\mathbf{k})k^2 = A_2(\mathbf{k}) \quad (17) \\ + \frac{1}{N} \sum_{\mathbf{q} \neq 0}^{(\pi)} a_3(\mathbf{k}, \mathbf{q})(q^2 + \mathbf{k}\mathbf{q}) + \frac{1}{2N} \sum_{\mathbf{q} \neq 0}^{(\pi)} q^2 a_4(\mathbf{q}, -\mathbf{q}, \mathbf{k}),$$

$$a_3(\mathbf{k}, \mathbf{q}) \approx A_3(\mathbf{k}, \mathbf{q}) - 2 \frac{R(\mathbf{k}, \mathbf{q})}{\epsilon_0(k) + \epsilon_0(q) + \epsilon_0(\mathbf{k} + \mathbf{q})}, \quad (18)$$

$$R(\mathbf{k}, \mathbf{q}) = \mathbf{k}\mathbf{q}a_2(\mathbf{k})a_2(\mathbf{q}) - \mathbf{k}(\mathbf{k} + \mathbf{q})a_2(\mathbf{k})a_2(\mathbf{k} + \mathbf{q}) \\ - \mathbf{q}(\mathbf{k} + \mathbf{q})a_2(\mathbf{q})a_2(\mathbf{k} + \mathbf{q}), \quad (19)$$

$$A_2(\mathbf{k}) = \frac{1}{\sqrt{N}} \sum_{q_x \neq 0}^{(2\pi)} ik_{cx} C_{l_x}(-q_x) \left[4(q_x + k_x) S_2^{(l)}(\mathbf{q}_x, \mathbf{k}) \right. \\ \left. + 6q_x S_3^{(l)}(\mathbf{q}_x, -\mathbf{q}_x, \mathbf{k}) \right] + (x \rightarrow y, z) \\ + \frac{1}{N} \sum_{\mathbf{q} \neq 0}^{(2\pi)} \left[4(q^2 + \mathbf{k}\mathbf{q}) S_1^{(l)}(-\mathbf{q}) S_2^{(l)}(\mathbf{q}, \mathbf{k}) + \right. \\ \left. + 4(\mathbf{k} + \mathbf{q})^2 S_2^{(l)}(\mathbf{q}, \mathbf{k}) S_2^{(l)}(-\mathbf{q}, -\mathbf{k}) \right. \\ \left. + 6q^2 S_1^{(l)}(-\mathbf{q}) S_3^{(l)}(\mathbf{q}, \mathbf{k}, -\mathbf{k}) \right], \quad (20)$$

where $\epsilon_0(\mathbf{k}) = k^2(1 - 2a_2(\mathbf{k}))$, $d = 3$ is the dimension of the system, and

$$\nu_3(k) = \int U_3(r) e^{-i\mathbf{k}\mathbf{r}} d\mathbf{r} \quad (21)$$

is the Fourier transform of the interaction potential $U_3(r)$ of two Bose particles. The equations for the functions $S_j^{(l)}$

can be obtained analogously from the equations for $S_j^{(1)}$ (see I):

$$S_1^{(l)}(\mathbf{q}) \epsilon_0(\mathbf{q}) = \\ = -i\sqrt{N} 2k_{cx} q_x a_2(-\mathbf{q}_x) C_{l_x}(q_x) \delta_{\mathbf{q}, \mathbf{q}_x} + (x \rightarrow y, z) \\ + \frac{1}{N} \sum_{\mathbf{q}_1 \neq 0}^{(\pi)} \left\{ 2(q_1^2 + \mathbf{q}_1 \mathbf{q}) S_2^{(l)}(\mathbf{q}, \mathbf{q}_1) + 6q_1^2 S_3^{(l)}(\mathbf{q}, \mathbf{q}_1, -\mathbf{q}_1) \right. \\ \left. + \sqrt{N} 4q_1^2 S_1^{(l)}(\mathbf{q}_1) S_2^{(l)}(\mathbf{q} - \mathbf{q}_1, \mathbf{q}_1) \right. \\ \left. + \sqrt{N} (q_1^2 - \mathbf{q}_1 \mathbf{q}) S_1^{(l)}(\mathbf{q}_1) S_1^{(l)}(\mathbf{q} - \mathbf{q}_1) \right\} \\ + \left\{ \sum_{p_x \neq 0}^{(2\pi)} 2ik_{cx} C_{l_x}(p_x) \left[(q_x - p_x) S_1^{(l)}(\mathbf{q} - \mathbf{p}_x) \right. \right. \\ \left. \left. - 2p_x S_2^{(l)}(\mathbf{q} - \mathbf{p}_x, -\mathbf{q}) \right] + (x \rightarrow y, z) \right\}, \quad (22)$$

$$S_2^{(l)}(\mathbf{q}, \mathbf{q}_1) [\epsilon_0(\mathbf{q}_1) + \epsilon_0(\mathbf{q} + \mathbf{q}_1)] \\ + 2S_1^{(l)}(\mathbf{q}) a_2(-\mathbf{q}_1) \mathbf{q}\mathbf{q}_1 - q^2 S_1^{(l)}(\mathbf{q}) a_3(\mathbf{q}, \mathbf{q}_1) \\ = \delta_{\mathbf{q}, \mathbf{q}_x} \sqrt{N} ik_{cx} C_{l_x}(q_x) \{ 2q_{1x} a_2(\mathbf{q}_1) - q_x a_3(\mathbf{q}_1, \mathbf{q}_x) \} \\ + \sum_{p_x \neq 0}^{(2\pi)} ik_{cx} C_{l_x}(p_x) \left[4(q_x + q_{1x} - p_x) S_2^{(l)}(\mathbf{q} - \mathbf{p}_x, \mathbf{q}_1) \right. \\ \left. - 6p_x S_3^{(l)}(\mathbf{q} - \mathbf{p}_x, \mathbf{q}_1, -\mathbf{q} - \mathbf{q}_1) \right] + (x \rightarrow y, z) \\ + \frac{1}{\sqrt{N}} \sum_{\mathbf{q}_2 \neq 0}^{(\pi)} \left\{ \frac{2}{\sqrt{N}} (q_2^2 - \mathbf{q}_1 \mathbf{q}_2) S_3^{(l)}(\mathbf{q}, \mathbf{q}_1 - \mathbf{q}_2, \mathbf{q}_2) \right. \\ \left. + \frac{4}{\sqrt{N}} \mathbf{q}_2(\mathbf{q}_1 + \mathbf{q}_2 + \mathbf{q}) S_3^{(l)}(\mathbf{q}, \mathbf{q}_1, \mathbf{q}_2) \right. \\ \left. - 4\mathbf{q}_2(\mathbf{q}_1 - \mathbf{q}_2 + \mathbf{q}) S_1^{(l)}(\mathbf{q}_2) S_2^{(l)}(\mathbf{q} - \mathbf{q}_2, \mathbf{q}_1) \right. \\ \left. + 6q_2^2 S_1^{(l)}(\mathbf{q}_2) S_3^{(l)}(\mathbf{q} - \mathbf{q}_2, \mathbf{q}_1, -\mathbf{q} - \mathbf{q}_1) \right. \\ \left. + 4(\mathbf{q}_1 + \mathbf{q}_2)^2 S_2^{(l)}(\mathbf{q}_2, \mathbf{q}_1) S_2^{(l)}(\mathbf{q} - \mathbf{q}_2, \mathbf{q}_1 + \mathbf{q}_2) \right\}. \quad (23)$$

Equations (14)–(23) are a complicated system of non-linear integral equations, whose solutions determine the properties of the ground state of the crystal with a rectangular lattice. Let us analyze these equations. Of a paramount interest are the value of E_0 and the distribution of atoms in the crystal.

It is seen from Eq. (22) that the nonzero value of $S_1^{(l)}(\mathbf{q})$ is determined by the first “one-dimensional” term $\sim C_{l_x}(q_x) \delta_{\mathbf{q}, \mathbf{q}_x}$ on the right-hand side. This yields the one-dimensional solutions $S_1^{(l)}(\mathbf{q}_x) \delta_{\mathbf{q}, \mathbf{q}_x}$, $S_1^{(l)}(\mathbf{q}_y) \delta_{\mathbf{q}, \mathbf{q}_y}$, and $S_1^{(l)}(\mathbf{q}_z) \delta_{\mathbf{q}, \mathbf{q}_z}$. However, the terms $\sim S_1^{(l)}(\mathbf{q}_1) S_2^{(l)}(\mathbf{q} - \mathbf{q}_1, \mathbf{q}_1)$ and some other ones on the right-hand side generate also not one-dimensional solutions of the form $S_1^{(l)}(\mathbf{q}_x + \mathbf{q}_y) \delta_{\mathbf{q}, \mathbf{q}_x + \mathbf{q}_y}$ and $S_1^{(l)}(\mathbf{q}_x + \mathbf{q}_y + \mathbf{q}_z)$ of the same order ($\sim \sqrt{N}$) as one-dimensional solutions. Since $C_{l_x}(j_x)$ are nonzero only at the “resonance” points $j_x = \pm l_x, \pm 2l_x, \pm 3l_x, \dots$, the function $S_1^{(l)}(\mathbf{q})$ is nonzero only

for the “resonance” wave vectors

$$\mathbf{q}^{res}(\mathbf{r}) = 2\pi \left(\frac{r_x l_x}{L_x}, \frac{r_y l_y}{L_y}, \frac{r_z l_z}{L_z} \right), \quad (24)$$

where $\mathbf{r} = (r_x, r_y, r_z)$, $r_x, r_y, r_z = \pm 1, \pm 2, \pm 3, \dots$. With regard for these relations, we can write the solution

$$\begin{aligned} S_1^{(1)}(\mathbf{q} = \mathbf{q}_x + \mathbf{q}_y + \mathbf{q}_z) &= S_1^{(1)}(\mathbf{q}) \left\{ \delta_{\mathbf{q}, \mathbf{q}_x^{res}} + \delta_{\mathbf{q}, \mathbf{q}_y^{res}} \right. \\ &+ \delta_{\mathbf{q}, \mathbf{q}_z^{res}} + \delta_{\mathbf{q}, \mathbf{q}_x^{res} + \mathbf{q}_y^{res}} + \delta_{\mathbf{q}, \mathbf{q}_x^{res} + \mathbf{q}_z^{res}} + \delta_{\mathbf{q}, \mathbf{q}_y^{res} + \mathbf{q}_z^{res}} \\ &\left. + \delta_{\mathbf{q}, \mathbf{q}_x^{res}} \right\} \end{aligned} \quad (25)$$

and, analogously, $S_{j \geq 2}^{(1)}(\mathbf{q}, \mathbf{q}_1, \dots, \mathbf{q}_{j-1})$. As is seen from Eq. (22), the values of $S_1^{(1)}(\mathbf{q}_x)$ depend significantly on the sums with $S_2^{(1)}$, $S_3^{(1)}$ and with the terms $\sim S_1^{(1)} S_1^{(1)}$, and $\sim S_1^{(1)} S_2^{(1)}$. However, we restrict ourselves to the zero approximation

$$S_1^{(1)}(\mathbf{q}_x) \approx -\frac{i\sqrt{N}2k_{cx}C_{l_x}(q_x)a_2(-\mathbf{q}_x)\delta_{\mathbf{q}_x, \mathbf{q}_x^{res}}}{q_x - 2q_x a_2(\mathbf{q}_x)}, \quad (26)$$

$$\begin{aligned} S_2^{(1)}(\mathbf{q}_x, \mathbf{q}_1) &\approx \delta_{\mathbf{q}_x, \mathbf{q}_x^{res}} \frac{i\sqrt{N}k_{cx}C_{l_x}(q_x)}{1 - 2a_2(\mathbf{q}_x)} \\ &\times \frac{2q_{1x}a_2(\mathbf{q}_1) - q_x a_3(\mathbf{q}_1, \mathbf{q}_x)}{\epsilon_0(\mathbf{q}_1) + \epsilon_0(\mathbf{q}_x + \mathbf{q}_1)}. \end{aligned} \quad (27)$$

The analogous relations are true for $S_1^{(1)}(\mathbf{q}_y)$, $S_1^{(1)}(\mathbf{q}_z)$ and $S_2^{(1)}(\mathbf{q}_y, \mathbf{q}_1)$, $S_2^{(1)}(\mathbf{q}_z, \mathbf{q}_1)$. The omitted corrections can renormalize $S_1^{(1)}(\mathbf{q}_x)$, by changing its value by several times. In this case, the higher corrections are damped by the decrease of $a_2(\mathbf{q})$ with increase in q . For the not one-dimensional solutions $S_1^{(1)}(\mathbf{q}_x + \mathbf{q}_y)$ and $S_1^{(1)}(\mathbf{q}_x + \mathbf{q}_y + \mathbf{q}_z)$, even the zero approximation is a complicated sum (over \mathbf{q}_1) of the terms $\sim S_1^{(1)}(\mathbf{q}_1)S_1^{(1)}(\mathbf{q} - \mathbf{q}_1)$ and $\sim S_1^{(1)}(\mathbf{q}_1)S_2^{(1)}(\mathbf{q} - \mathbf{q}_1, \mathbf{q}_1)$. By our estimates, the not one-dimensional solutions are significantly less than the one-dimensional ones. Due to the complexity of the equations, we neglect the not one-dimensional solutions:

$$S_1^{(1)}(\mathbf{q}) \simeq S_1^{(1)}(\mathbf{q}) \left\{ \delta_{\mathbf{q}, \mathbf{q}_x^{res}} + \delta_{\mathbf{q}, \mathbf{q}_y^{res}} + \delta_{\mathbf{q}, \mathbf{q}_z^{res}} \right\}. \quad (28)$$

Let us study the distribution of atoms along the x -axis (coinciding with one of the axes of a crystal) for the lattice of He^4 atoms at $\bar{R}_x = \bar{R}_y = \bar{R}_z = \bar{R} = 3.6 \text{ \AA}$. According to I, the probability for an atom to be at a point x is approximately determined by the formulas

$$\psi(x) \simeq \sin(k_{cx}x)e^{s_1(x)}, \quad (29)$$

$$s_1(x) \simeq \sum_{q_x = 2\pi j_x / L_x}^{(2\pi)} \frac{S_1^{(1)}(\mathbf{q}_x)}{\sqrt{N}} e^{iq_x x}, \quad (30)$$

where $j_x = \pm 1, \pm 2, \pm 3, \dots$ and $k_{cx} = \pi/\bar{R}$. Despite the approximate character of the formulas, we may expect that they give the general form of a probability distribution in a cell.

Since $S_1^{(1)}(\mathbf{q}_x) \neq 0$ only at the resonance points and $S_1^{(1)}(-\mathbf{q}_x) = S_1^{(1)}(\mathbf{q}_x)$, we have

$$s_1(x) \simeq \sum_{r_x=1,2,\dots} \frac{S_1^{(1)}(\mathbf{q}_x)}{\sqrt{N}} 2 \cos(q_x x), \quad (31)$$

where $q_x = r_x 2\pi l_x / L_x = r_x 2\pi / \bar{R}$. We will determine $S_1^{(1)}(\mathbf{q}_x)$ from Eq. (26), by using the zero approximation for $a_2(q)$,

$$a_2(q) = \frac{1}{2} - \sqrt{\frac{1}{4} + \frac{n\nu_3(q)m}{8\hbar^2 q^2}}, \quad (32)$$

which follows from (17) if all sums are neglected. Note that we took the solution with the sign “minus” before the root (see I).

We choose the interatomic interaction potential for atoms of the crystal, as in I:

$$U_3(\mathbf{r}) \approx \begin{cases} U_b & r \leq a \\ U_{bd} & a \leq r \leq b \\ 0 & r > b. \end{cases} \quad (33)$$

Below, we use, unless otherwise indicated, $a = 2 \text{ \AA}$, $b = 4 \text{ \AA}$, $U_{bd} = -9 \text{ K}$, which corresponds approximately to He^4 atoms. This potential is sufficiently crude, but it is qualitatively proper and has the analytical Fourier transform

$$\nu_3(k) = \frac{4\pi}{k^3} \tilde{\nu}_3(k), \quad (34)$$

$$\begin{aligned} \tilde{\nu}_3(k) &= [U_b - U_{bd}][\sin(ak) - ak \cos(ak)] \\ &+ U_{bd}[\sin(bk) - bk \cos(bk)]. \end{aligned} \quad (35)$$

By formulas (29)–(35), we determine $\psi(x)$ (29). It has a periodic shape, in correspondence with the domain structure. The distribution $|\psi(x)|^2$ in one of the domains is shown in Fig. 1. The value of \bar{R} is chosen like that for He II: $\bar{R} = 3.6 \text{ \AA}$, which is close to \bar{R} of the crystalline phases of He^4 . As is seen from Fig. 1, the distribution $|\psi(x)|^2$ at the height of the potential barrier $U_b = 300 \text{ K}$ is similar to the bare one ($\sin^2(k_{cx}x)$), but is more flattened. At $U_b \gtrsim 1000 \text{ K}$, we see the appearance of two maxima located symmetrically relative to the center of a cell. They increase with U_b . So, the probability density is the highest not at the center of a cell, as is commonly accepted, but at these maxima. In the three-dimensional case, the maxima indicate the presence, inside a cell, of an orbit with cubic shape. The orbit depends on the values of a and b : at $a = 1 \text{ \AA}$, $b = 3 \text{ \AA}$ and $U_b = 3000 \text{ K}$, the maxima disappear, and $|\psi(x)|^2$ is similar to the curve of triangles in Fig. 1. But such small a does not correspond

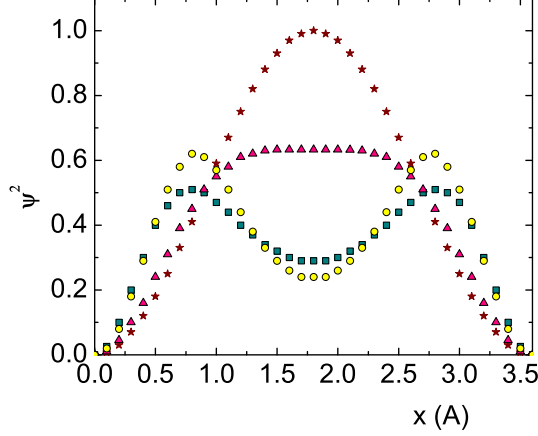


Fig. 1: Probability density $|\psi(x)|^2$ (29), (31) versus the coordinate x of a cell of the sc crystal at the potential with $a = 2 \text{ \AA}$, $b = 4 \text{ \AA}$, $U_{bd} = -9 \text{ K}$ and the barriers $U_b = 300 \text{ K}$ (triangles), $U_b = 3000 \text{ K}$ (circles), and $U_b = 3000 \text{ K}$ with regard for only the first term in sum (31) (squares). Stars stand for the bare function $\sin^2(k_{cx}x)$. The x -axis coincides with the x -axis of a cell of the crystal, values of x are given in \AA .

to the He^4 - He^4 potential. As a increases by 1 \AA , there appears a clear orbit, like the curve of circles in Fig. 1.

The orbit size is approximately equal to a half of the cell size, because the main contribution to the maxima is given by the first term (with $q_x = 2k_{cx}$) in sum (31). The terms with $q_x = 4k_{cx}, 6k_{cx}, 8k_{cx}$ are small, and the peaks for $q_x = 4k_{cx}$ arise only at $U_b \gtrsim 10^6 \text{ K}$ (see Fig. 2). To calculate $|\psi(x)|^2$, it is sufficient to take two first terms in sum (31) (due to the fast decrease of $a_2(q)$, as q increases).

In Fig. 2, we present the dependence of the orbit on the barrier height U_b . As is seen, the orbit becomes narrow at large U_b . Moreover, at $U_b = 10^6 \text{ K}$ and 10^7 K , the second orbit appears at a distance of $\simeq 0.5 \text{ \AA}$ from the wall of a cell. However, the neglected higher correlative corrections become large at large U_b , which can lead to the widening of orbits.

In Fig. 2, stars show $|\psi(x)|^2$ for the lattice of krypton atoms. The orbit is narrow at the barrier $U_b = 3000 \text{ K}$, whereas the orbit for helium atoms is wide at such U_b . However, it is known^{1,35} that the ground state of the crystal of heavy inert elements is well described under the assumption of small oscillations of atoms near points of the lattice. Apparently, there is no contradiction in this case, since the function $r^2|\psi(r)|^2$ at small oscillations is characterized by a spherical orbit¹ with approximately the same size. Nevertheless, the orbit in Fig. 2 has shape of the surface of a cube (with edge $\bar{R}/2$), rather than a sphere, even for the function $r^2|\psi(r)|^2$. In other words, the motion of an atom is oscillatory only approximately. More exactly, this motion has a wave character. This fact is unusual and means that the resonance wave (the

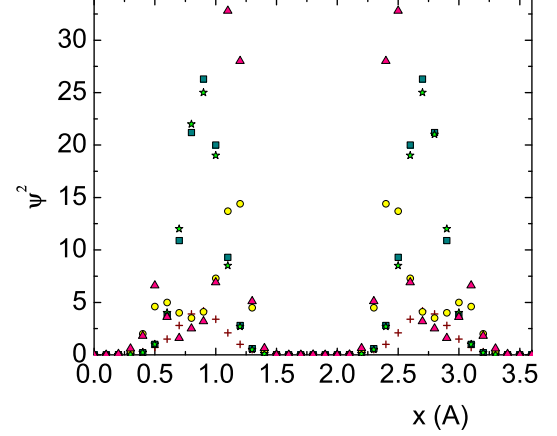


Fig. 2: Function $|\psi(x)|^2$ for a sc crystal of He^4 at high barriers U_b . Potential (33) with $a = 2 \text{ \AA}$, $b = 4 \text{ \AA}$, $U_{bd} = -9 \text{ K}$ and the barriers $U_b = 9000 \text{ K}$ (crosses), $U_b = 10^5 \text{ K}$ (squares), $U_b = 10^6 \text{ K}$ (circles) and $U_b = 10^7 \text{ K}$ (triangles). Stars mark the curve for a crystal of krypton atoms with the same parameters except the mass ($m = 21m_4$) and potential ($U_b = 3000 \text{ K}$, $U_{bd} = -140 \text{ K}$).

product of sines in (2)) sets the lattice of a crystal and the motion of atoms in the cells.

Can an orbit be discovered in experiments? The scattering of light or neutrons in a crystal will show ordinary Bragg-Wolf peaks first of all, since the time average of the positions of an atom is the center of a cell. But the orbit can be revealed in some specific features of the scattering.

Let us estimate the ground-state energy E_0 of a sc crystal, using formulas (14)–(17). With regard for solution (28) for $S_1^{(1)}(\mathbf{q})$ with $S_1^{(1)}(\mathbf{q}_x)$ (26) and solution (13) for $C_l(j)$, we obtain

$$E_0 = \tilde{E}_0^b + A_1, \quad A_1 = \frac{\hbar^2 k_c^2}{2m} \left[1 + 8 \sum_r \frac{a_2(q_x) - 3a_2^2(q_x)}{(2a_2(q_x) - 1)^2} \right], \quad (36)$$

where $r = 1, 2, 3, \dots$, $q_x = 2\pi r/\bar{R}$, $k_c^2 = 3\pi^2/\bar{R}^2$, and \tilde{E}_0^b (16) coincides with E_0 of a Bose fluid. Consider a crystal of He^4 atoms with $\bar{R} = 3.6 \text{ \AA}$, $\hbar^2 k_c^2/2m \approx 13.85 \text{ K}$, and the potential (33) with $a = 2 \text{ \AA}$, $b = 4 \text{ \AA}$, $U_{bd} = -9 \text{ K}$. Using the zero approximation (32) for $a_2(q_x)$ and taking the barrier $U_b = 1000 \text{ K}$, we obtain $A_1 \approx -12 \text{ K}$, $E_0 \approx -430 \text{ K}$. For $U_b = 200 \text{ K}$, we have $A_1 \approx 4 \text{ K}$, $E_0 \approx -36 \text{ K}$, whereas $A_1 \approx 9 \text{ K}$, $E_0 \approx -1 \text{ K}$ for $U_b = 81 \text{ K}$. The last value of E_0 is close to the experimental one¹. For He II, E_0 corresponds to experimental data also for $U_b \sim 100 \text{ K}$ (see I). For the realistic value $U_b \sim 10^3 - 10^4 \text{ K}$, the experimental value $E_0 \simeq -1 \text{ K}$ can be obtained with regard for correlative corrections.

The most essential and unexpected is the conclusion that the lattice is created by a standing wave in the probability field. As we see in Sec. 3, this wave is similar to

a sound one. In other words, the crystals have a wave nature.

III. STATE WITH A LONGITUDINAL ACOUSTIC PHONON

Consider a crystal with sc lattice. An optical phonons are absent for it. We consider only longitudinal acoustic phonons. The WF of a crystal with a single phonon can be obtained from the solution for a one-phonon state of the Bose fluid (see I) by the following changes: $\mathbf{k}_1 \rightarrow \mathbf{k}_c$, $C_1(q) \rightarrow C_l(q)$, and $S_j^{(1)} \rightarrow S_j^{(l)}$. We obtain

$$\Psi_{\mathbf{k}}(\mathbf{r}_1, \dots, \mathbf{r}_N) = \psi_{\mathbf{k}} \Psi_0, \quad (37)$$

$$\psi_{\mathbf{k}} = \psi_{\mathbf{k}}^0 + 7 \text{ permutations}, \quad (38)$$

$$\begin{aligned} \psi_{\mathbf{k}}^0 &= \psi_{\mathbf{k}}^b + b_0(\mathbf{k}) + \sum_{\mathbf{q} \neq 0, -\mathbf{k}}^{(2\pi)} Q_1(\mathbf{q}, \mathbf{k}) \rho_{-\mathbf{q}-\mathbf{k}} \\ &+ \sum_{\mathbf{q}, \mathbf{q}_1 \neq 0}^{\mathbf{q}+\mathbf{q}_1+\mathbf{k} \neq 0} \frac{Q_2(\mathbf{q}, \mathbf{q}_1, \mathbf{k})}{\sqrt{N}} \rho_{\mathbf{q}_1} \rho_{-\mathbf{q}-\mathbf{q}_1-\mathbf{k}} \\ &+ \sum_{\mathbf{q}, \mathbf{q}_1, \mathbf{q}_2 \neq 0}^{\mathbf{q}+\mathbf{q}_1+\mathbf{q}_2+\mathbf{k} \neq 0} \frac{Q_3(\mathbf{q}, \mathbf{q}_1, \mathbf{q}_2, \mathbf{k})}{N} \rho_{\mathbf{q}_1} \rho_{\mathbf{q}_2} \rho_{-\mathbf{q}-\mathbf{q}_1-\mathbf{q}_2-\mathbf{k}} + \dots, \end{aligned} \quad (39)$$

$$\begin{aligned} \psi_{\mathbf{k}}^b &= \rho_{-\mathbf{k}} + \sum_{\mathbf{k}_2 \neq 0, -\mathbf{k}}^{(\pi)} \frac{b_2(\mathbf{k}_2, \mathbf{k})}{\sqrt{N}} \rho_{\mathbf{k}_2} \rho_{-\mathbf{k}_2-\mathbf{k}} \\ &+ \sum_{\mathbf{k}_2, \mathbf{k}_3 \neq 0}^{(\pi) \mathbf{k}_2+\mathbf{k}_3+\mathbf{k} \neq 0} \frac{b_3(\mathbf{k}_2, \mathbf{k}_3, \mathbf{k})}{N} \rho_{\mathbf{k}_2} \rho_{\mathbf{k}_3} \rho_{-\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}} + \dots, \end{aligned} \quad (40)$$

where the permutation means $\psi_{\mathbf{k}}^0$ with the different sign of one or several components of the vector \mathbf{k} , the vector \mathbf{q} is quantized like $2\pi j/L$, and the vectors \mathbf{k}_j , \mathbf{q}_j , and \mathbf{k} are quantized like $\pi j/L$.

Solution (38) describes a three-dimensional standing wave decaying into eight counter traveling waves.

The energy of a phonon $E(k)$ and the functions b_j , Q_j

satisfy the equations

$$\begin{aligned} \epsilon(k) &= \epsilon_0(k) - \frac{1}{N} \sum_{\mathbf{k}_2 \neq 0}^{(\pi)} b_2(\mathbf{k}_2, \mathbf{k}) 2\mathbf{k}_2(\mathbf{k}_2 + \mathbf{k}) \\ &- \frac{1}{N} \sum_{\mathbf{k}_2 \neq 0}^{(\pi)} 6k_2^2 b_3(\mathbf{k}_2, -\mathbf{k}_2, \mathbf{k}) \\ &- \frac{2}{\sqrt{N}} \sum_{\mathbf{q} \neq 0}^{(2\pi)} Q_1(\mathbf{q}, \mathbf{k})(\mathbf{k} + \mathbf{q}) \\ &\times \left[\mathbf{q} S_1^{(l)}(-\mathbf{q}) + 2(\mathbf{k} + \mathbf{q}) S_2^{(l)}(-\mathbf{q}, -\mathbf{k}) \right] \\ &- \frac{4}{\sqrt{N}} \sum_{\mathbf{q} \neq 0}^{(2\pi)} q^2 Q_2(-\mathbf{q}, \mathbf{q}, \mathbf{k}) S_1^{(l)}(\mathbf{q}) \\ &- \sum_{q_x \neq 0}^{(2\pi)} 2k_{cx}(k_x + q_x) i C_{l_x}(-q_x) Q_1(\mathbf{q}_x, \mathbf{k}) \\ &+ \sum_{q_x \neq 0}^{(2\pi)} 4k_{cx} q_x i C_{l_x}(q_x) Q_2(-\mathbf{q}_x, \mathbf{q}_x, \mathbf{k}) + (x \rightarrow y, z), \end{aligned} \quad (41)$$

$$\begin{aligned} &Q_1(\mathbf{q}, \mathbf{k}) [\epsilon(k) - \epsilon_0(\mathbf{k} + \mathbf{q})] = \\ &= 2ik_{cx} C_{l_x}(q_x) \delta_{\mathbf{q}, \mathbf{q}_x} [-k_x + 2q_x b_2(\mathbf{q}, \mathbf{k})] \\ &+ \frac{2S_1^{(l)}(\mathbf{q})}{\sqrt{N}} [\mathbf{q}\mathbf{k} - 2q^2 b_2(\mathbf{q}, \mathbf{k})] - \frac{4k^2}{\sqrt{N}} S_2^{(l)}(\mathbf{q}, -\mathbf{q} - \mathbf{k}) \\ &- \frac{1}{N} \sum_{\mathbf{q}_1 \neq 0}^{(\pi)} \{ 2\mathbf{q}_1(\mathbf{q}_1 + \mathbf{q} + \mathbf{k}) \\ &\times [Q_2(\mathbf{q}, \mathbf{q}_1, \mathbf{k}) + Q_1(\mathbf{q} + \mathbf{q}_1, \mathbf{k}) \sqrt{N} S_1^{(l)}(-\mathbf{q}_1)] \\ &+ 6q_1^2 Q_3(\mathbf{q}, \mathbf{q}_1, -\mathbf{q}_1, \mathbf{k}) \\ &+ 4q_1^2 Q_2(\mathbf{q} - \mathbf{q}_1, \mathbf{q}_1, \mathbf{k}) \sqrt{N} S_1^{(l)}(\mathbf{q}_1) \\ &+ 4(\mathbf{q}_1 + \mathbf{q} + \mathbf{k})^2 Q_1(\mathbf{q} + \mathbf{q}_1, \mathbf{k}) \sqrt{N} S_2^{(l)}(-\mathbf{q}_1, -\mathbf{q} - \mathbf{k}) \} \\ &+ \sum_{p_x \neq 0}^{(2\pi)} 2k_{cx} i C_{l_x}(p_x) [(-k_x - q_x + p_x) Q_1(\mathbf{q} - \mathbf{p}_x, \mathbf{k}) \\ &+ 2p_x Q_2(\mathbf{q} - \mathbf{p}_x, \mathbf{p}_x, \mathbf{k})] + (x \rightarrow y, z), \end{aligned} \quad (42)$$

$$\begin{aligned} b_0(\mathbf{k}) \epsilon(k) &= -2k^2 S_1^{(l)}(-\mathbf{k}) \delta_{\mathbf{k}, \mathbf{k}^e} \\ &- 2k_{cx} k_x i C_{l_x}(-k_x) \sqrt{N} \delta_{\mathbf{k}, \mathbf{k}_x^e} \\ &- \frac{2}{\sqrt{N}} \sum_{\mathbf{q} \neq 0}^{(\pi)} q^2 Q_2(-\mathbf{k}, \mathbf{q}, \mathbf{k}) \delta_{\mathbf{k}, \mathbf{k}^e} \\ &- \sum_{\mathbf{q} \neq 0, -\mathbf{k}}^{(2\pi)} 2(\mathbf{k} + \mathbf{q})^2 Q_1(\mathbf{q}, \mathbf{k}) S_1^{(l)}(-\mathbf{k} - \mathbf{q}) \delta_{\mathbf{k}, \mathbf{k}^e} \\ &+ \sum_{q_x \neq 0}^{(2\pi)} 2\sqrt{N} k_{cx} q_x i C_{l_x}(q_x) Q_1(-\mathbf{k} - \mathbf{q}_x, \mathbf{k}) \delta_{\mathbf{k}, \mathbf{k}^e} \\ &+ (x \rightarrow y, z), \end{aligned} \quad (43)$$

$$\begin{aligned}
& b_2(\mathbf{k}_2, \mathbf{k}) [\epsilon(k) - \epsilon_0(\mathbf{k}_2) - \epsilon_0(\mathbf{k} + \mathbf{k}_2)] = \\
& = \mathbf{k}\mathbf{k}_2 a_2(\mathbf{k}_2) - \mathbf{k}(\mathbf{k} + \mathbf{k}_2) a_2(\mathbf{k} + \mathbf{k}_2) - k^2 a_3(\mathbf{k}, \mathbf{k}_2) \\
& - \frac{2}{\sqrt{N}} \sum_{\mathbf{k}_3 \neq 0}^{(\pi)} \left\{ \frac{3\mathbf{k}_3(\mathbf{k}_2 + \mathbf{k}_3 + \mathbf{k})}{\sqrt{N}} b_3(\mathbf{k}_2, \mathbf{k}_3, \mathbf{k}) \right. \\
& + Q_1(\mathbf{k}_3, \mathbf{k})(\mathbf{k}_3 + \mathbf{k}) \left[2(\mathbf{k}_3 - \mathbf{k}_2) S_2^{(1)}(-\mathbf{k}_3, \mathbf{k}_2) \right. \\
& + 3(\mathbf{k}_3 + \mathbf{k}) S_3^{(1)}(-\mathbf{k}_3, \mathbf{k}_2, -\mathbf{k}_2 - \mathbf{k}) \left. \right] \\
& + 2Q_2(-\mathbf{k}_3, \mathbf{k}_2 + \mathbf{k}_3, \mathbf{k})(\mathbf{k}_2 + \mathbf{k}_3) \\
& \times \left[\mathbf{k}_3 S_1^{(1)}(\mathbf{k}_3) + 2(\mathbf{k}_2 + \mathbf{k}_3) S_2^{(1)}(\mathbf{k}_3, \mathbf{k}_2) \right] \\
& + 3k_3^2 S_1^{(1)}(\mathbf{k}_3) Q_3(-\mathbf{k}_3, \mathbf{k}_2, -\mathbf{k}_2 - \mathbf{k}, \mathbf{k}) \left. \right\} \\
& + \sum_{p_x \neq 0}^{(2\pi)} 2k_{cx} i C_{l_x}(p_x) [3p_x Q_3(-\mathbf{p}_x, \mathbf{k}_2, -\mathbf{k}_2 - \mathbf{k}, \mathbf{k}) \\
& + 2(k_{2x} + p_x) Q_2(-\mathbf{p}_x, \mathbf{k}_2 + \mathbf{p}_x, \mathbf{k})], \\
& + \text{higher corrections} + (x \rightarrow y, z), \tag{44}
\end{aligned}$$

where $\epsilon(k) = 2mE(k)/\hbar^2$, \mathbf{k}^e is the wave vector with all even components (i.e., they are multiple to $2\pi/L$), $\mathbf{q}_x = q_x \mathbf{i}_x$, and $\mathbf{p}_x = p_x \mathbf{i}_x$. By $(x \rightarrow y, z)$, we denote the same terms as one with the separated x -component, but with the changes $x \rightarrow y$ and $x \rightarrow z$. All terms of Eqs. (41)–(44), except for the first one, contain a product of two wave vectors (for example, q^2 , $k_{cx}k_x$, or $(\mathbf{k}_3 + \mathbf{k})(\mathbf{k}_3 - \mathbf{k}_2)$). These wave vectors must be nonzero.

Some of these equations contain the sums, where the first argument of the functions Q_l or $S_j^{(1)}$ has components multiple to π/L . In this case, we set $Q_l = 0$, $S_j^{(1)} = 0$, because, by the definition of these functions, the components of the first argument are multiple to $2\pi/L$.

Equations (41)–(44) are written in the approximation of “two sums in the wave vector”, at which the series contain the functions a_2 , a_3 , b_2 , b_3 , $S_{j \leq 3}^{(1)}$, and $Q_{l \leq 3}$ and do not include the corrections $a_{j \geq 4}$, $b_{j \geq 4}$, $S_{j \geq 4}^{(1)}$, and $Q_{l \geq 4}$.

It follows from Eq. (42) that the solution for the function $Q_1(\mathbf{q}, \mathbf{k})$ has a “resonance” form analogous to (25). We restrict ourselves to the one-dimensional approximation:

$$Q_1^{(1)}(\mathbf{q}, \mathbf{k}) \simeq Q_1^{(1)}(\mathbf{q}, \mathbf{k}) \left\{ \delta_{\mathbf{q}, \mathbf{q}_x^{res}} + \delta_{\mathbf{q}, \mathbf{q}_y^{res}} + \delta_{\mathbf{q}, \mathbf{q}_z^{res}} \right\}. \tag{45}$$

In the zero approximation without regard for the sums in Eq. (42), we have

$$\begin{aligned}
Q_1(\mathbf{q}_x, \mathbf{k}) &= \left[2ik_{cx} C_{l_x}(q_x) - 2q_x S_1^{(1)}(\mathbf{q}_x) / \sqrt{N} \right] \\
&\times \frac{-k_x + 2q_x b_2(\mathbf{q}_x, \mathbf{k})}{\epsilon(k) - \epsilon_0(\mathbf{k} + \mathbf{q}_x)} \\
&\approx \frac{i2k_{cx} C_{l_x}(q_x)}{1 - 2a_2(q_x)} \times \frac{-k_x + 2q_x b_2(\mathbf{q}_x, \mathbf{k})}{\epsilon(k) - \epsilon_0(\mathbf{k} + \mathbf{q}_x)}. \tag{46}
\end{aligned}$$

The analogous relations can be given for $Q_1(\mathbf{q}_y, \mathbf{k})$, and $Q_1(\mathbf{q}_z, \mathbf{k})$.

Equations (41)–(44) are very complicated. By setting $Q_l = 0$ in them, we obtain the equations for a Bose fluid, namely, for b_2 and the dispersion curve $E(k)$. Thus, the equations for a crystal are the equations for a fluid plus some additional anisotropic corrections.

Let us consider dispersion curves. First, the value of b_0 does not influence $E(k)$. In the simplest approximation with regard for the anisotropy, the dispersion curves are determined by the formula

$$\begin{aligned}
\epsilon(\mathbf{k}) &= \epsilon_0(k) - \frac{2}{\sqrt{N}} \sum_{\mathbf{q} \neq 0}^{(2\pi)} Q_1(\mathbf{q}, \mathbf{k})(\mathbf{k} + \mathbf{q}) \mathbf{q} S_1^{(1)}(-\mathbf{q}) \\
&- \sum_{q_x \neq 0}^{(2\pi)} 2k_{cx}(k_x + q_x) i C_{l_x}(-q_x) Q_1(\mathbf{q}_x, \mathbf{k}) \\
&+ (x \rightarrow y, z). \tag{47}
\end{aligned}$$

With regard for solutions (13), (26), (28), (45), and (46) in the approximation $b_2 = 0$, we obtain

$$\epsilon(\mathbf{k}) = \epsilon_0(k) + \epsilon_x^{cr}(\mathbf{k}) + \epsilon_y^{cr}(\mathbf{k}) + \epsilon_z^{cr}(\mathbf{k}), \tag{48}$$

$$\epsilon_x^{cr}(\mathbf{k}) = - \sum_{q_x = q_x^{res}} \frac{4k_{cx}^2}{(1 - 2a_2(q_x))^2} \frac{k_x(k_x + q_x)}{\epsilon(\mathbf{k}) - \epsilon_0(\mathbf{k} + \mathbf{q}_x)}, \tag{49}$$

where the sum is taken over the resonance values of $q_x^{res} = \pm 2k_{cx}, \pm 4k_{cx}, \pm 6k_{cx}, \dots$. For a sc crystal,

$$E(\mathbf{k}) = \frac{\hbar^2 \epsilon_0(\mathbf{k})}{2m} + j \frac{\hbar^2 \epsilon_x^{cr}(\mathbf{k})}{2m}, \tag{50}$$

where $j=1, 2$, and 3 for directions $(1,0,0)$, $(1,1,0)$, and $(1,1,1)$. Since the values of $\epsilon_x^{cr}(\mathbf{k})$ and $\epsilon_0(k)$ are of the same order, the dispersion curves are different for different directions. In other words, the spectrum of longitudinal acoustic phonons is anisotropic, what was observed in experiments.

Due to a large value of ϵ_x^{cr} , the method of iterations does not converge, and the more exact numerical methods require much time for the analysis. To demonstrate the influence of the correction ϵ_x^{cr} , we decrease it by two orders of magnitude so that the method of iterations can be applied. In Fig. 3, we present the dispersion curves calculated by formula (50). The curves are different for different directions and are similar to the observed ones² for a bcc crystal of He^4 .

The qualitative behavior of the dispersion curves can be understood, by using the simple formula

$$E(\mathbf{k}) \approx \frac{\hbar^2 \epsilon_0(\mathbf{k})}{2m} = \frac{\hbar^2 k^2}{2m} (1 - 2a_2(\mathbf{k})). \tag{51}$$

With regard for approximation (32) for $a_2(\mathbf{k})$, this formula becomes

$$E(k) \approx \sqrt{\left(\frac{\hbar^2 k^2}{2m} \right)^2 + \frac{n\nu_3(k)}{8} \frac{\hbar^2 k^2}{m}}. \tag{52}$$

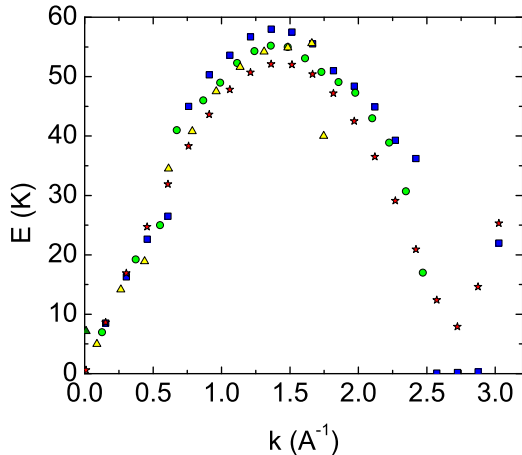


Fig. 3: Dispersion curves $E(\mathbf{k})$ (50) with ϵ_x^{cr} decreased by two orders of magnitude for directions (1,0,0) (triangles), (1,1,0) (circles), and (1,1,1) (squares) for a sc crystal of He^4 atoms with $\bar{R} = 3.6 \text{ \AA}$ and potential (33) with $a = 2 \text{ \AA}$, $b = 4 \text{ \AA}$, $U_{bd} = -9 \text{ K}$ and $U_b = 3000 \text{ K}$. Stars show the zero approximation $E(\mathbf{k}) = \hbar^2 \epsilon_0(k)/2m$. For the comparison with experiments, the dispersion curves are drawn to k^{max} of the bcc lattice.

It is the well-known Bogolyubov formula with the additional multiplier $1/8$ arising due to the boundaries (see I). Indeed, for each of the directions (1,0,0), (1,1,0), and (1,1,1), we need to continue curve (52) to k^{max} for a given direction. We obtained no anisotropy, but the general shape of the curve is proper: the phonon curve has no minimum for direction (1,0,0), a slightly pronounced minimum for (1,1,0), and a clear minimum for (1,1,1). This corresponds to experiments² for the bcc lattice of He^4 . The minimum arise due to a displacement of k^{max} to the side of large k and to the presence of a minimum on the liquid-like curve $E(\mathbf{k}) = \hbar^2 \epsilon_0(k)/2m$. To describe the curve more exactly and to obtain the anisotropy, we need to consider the next corrections to the equations.

It is of interest that the simple formula (52) describes the curves qualitatively correctly. This formula is universal and is valid for a gas, a liquid, and a crystal, since these three states of substance are described by WFs with the same structure (2), (37)–(40) (the difference is only in the values of \mathbf{k}_1).

The theoretical dispersion curves for a crystal and He II (see I) correspond to the experiment at $U_b \sim 10^3 \text{ K}$. For E_0 , the agreement with experiment for a liquid and a crystal holds at $U_b \sim 10^2 \text{ K}$ (see Sec. 2). However, it is assumed that the best potential for He^4 atoms is the Aziz potential³⁶ with much more larger value of U_b , about $2 \times 10^6 \text{ K}$. This disagreement is related to the neglect of higher corrections or (more probably) to the fact that the potential at small distances has only an effective meaning. Therefore, the values of U_b can be very different for different processes. In some models, the agreement with experiment was attained with the Aziz potential.

In Fig. 3, the dispersion curves are broken at k^{max} equal to a half of the minimum vector \mathbf{g}_0 of the reciprocal lattice (for directions (1,0,0), (1,1,0), and (1,1,1) of a sc crystal, $\mathbf{g}_0 = \pi(1/\bar{R}, 0, 0)$, $\pi(1/\bar{R}, 1/\bar{R}, 0)$ and $\pi(1/\bar{R}, 1/\bar{R}, 1/\bar{R})$, whereas \mathbf{g}_0 is twice larger for the bcc lattice), since the dispersion curves for crystals are periodic with period \mathbf{g} :

$$E(\mathbf{k} + \mathbf{g}) = E(\mathbf{k}). \quad (53)$$

The proof of this fact for one-particle WFs³⁷ can be easily generalized to our case of N -particle WFs. However, it is true for the cyclic BCs. For a three-dimensional crystal, the BCs are quite different and are close to zero ones. However, the majority of quasiparticles are localized wave packets (this is supported by the fact that the theory of transfer was constructed for wave packets and agrees with experiment). For such packets, the translational invariance with the period of a lattice holds, and the conclusions of the theorem are valid. As for the standing waves (37)–(40), they are the sum of eight traveling waves, from which the wave packets can be constructed.

We note that the density of phonon states at the quantization of \mathbf{k} by law (5) is the same as that for cyclic BCs.

In the literature^{1,38,39}, the dispersion curves of crystals are usually calculated in the approximation of small oscillations (1).

IV. THE CONDENSATE

In Ref. 40 and recently⁴¹, it was shown that the ideal crystal in the ground state contains no condensate atoms with $\mathbf{k} = 0$. However, the condensate is possible in the presence of vacancies and other defects^{17,20–22,24,26}. The condensate can be a key factor for the explanation of NCIM. But the experiment does not confirm⁴² a condensate of atoms with $\mathbf{k} = 0$.

It follows from Ψ_0 (2) that the ideal sc crystal does not possess off-diagonal long-range order, but it have a condensate of atoms with $\mathbf{k} = \mathbf{k}_1$. It is easy to verify if we switch-off the interatomic interaction: in this case, the exponents in Ψ_0 (2) become equal to 1, and we have the product of sines with $\mathbf{k} = \mathbf{k}_1$, i.e., all atoms are in the condensate with $\mathbf{k} = \mathbf{k}_1$. If the interaction is switched-on, the condensate is exhausted. For a fluid, the condensate is also determined by a factor before the exponential function: under cyclic BCs, this factor ($\prod_j e^{i\mathbf{p} \cdot \mathbf{r}_j} |_{\mathbf{p}=0} = 1$) generates the condensate of atoms with $\mathbf{p} = 0$. For the fluid in a vessel, the factor is the product of sines with $\mathbf{k} = \mathbf{k}_1$ (see I), and the condensate is on the levels with $\mathbf{k} = \mathbf{k}_1, 3\mathbf{k}_1, 5\mathbf{k}_1, \dots$ ⁴³.

Let us calculate the condensate for the ground state of a sc crystal. Under zero BCs, the condensate is deter-

mined by the formula⁴³

$$\frac{N_{\mathbf{k}_n}}{N} = \frac{8}{V^2} \int_0^{L_x, L_y, L_z} d\mathbf{r}_1 d\mathbf{r}_2 \rho(\mathbf{r}_1, \mathbf{r}_2) \sin(k_{n_x} x_1) \sin(k_{n_x} x_2) \times \sin(k_{n_y} y_1) \sin(k_{n_y} y_2) \sin(k_{n_z} z_1) \sin(k_{n_z} z_2), \quad (54)$$

$$\rho(\mathbf{r}_a, \mathbf{r}_b) = V \int d\mathbf{r} \Psi_0^*(\mathbf{r}_a, \mathbf{r}) \Psi_0(\mathbf{r}_b, \mathbf{r}), \quad (55)$$

where n_x, n_y, n_z are integers, $\mathbf{n} = (n_x, n_y, n_z)$, and \mathbf{r} marks a collection of vectors $\mathbf{r}_2, \dots, \mathbf{r}_N$. Relation (2) yields

$$\begin{aligned} \rho(\mathbf{r}_a, \mathbf{r}_b) &= \sin(k_{l_x} x_a) \sin(k_{l_y} y_a) \sin(k_{l_z} z_a) \\ &\times \sin(k_{l_x} x_b) \sin(k_{l_y} y_b) \sin(k_{l_z} z_b) \\ &\times |A|^2 V \int d\mathbf{r} \left[\exp \left\{ (S_w^{(1)}(\mathbf{r}_a, \mathbf{r}))^* \right\} \right. \\ &\times \exp \left\{ S_w^{(1)}(\mathbf{r}_b, \mathbf{r}) + \tilde{S}_b(\mathbf{r}_a, \mathbf{r}) + \tilde{S}_b(\mathbf{r}_b, \mathbf{r}) \right\} \\ &\times \left. \prod_{j=2}^N \{ \sin^2(k_{l_x} x_j) \sin^2(k_{l_y} y_j) \sin^2(k_{l_z} z_j) \} \right]. \end{aligned} \quad (56)$$

In $S_w^{(1)}$ (6), we consider only the one-particle part $S_1^{(1)}$. Then

$$\begin{aligned} \rho(\mathbf{r}_a, \mathbf{r}_b) &= \rho_\infty^c \sin(k_{l_x} x_a) \sin(k_{l_y} y_a) \sin(k_{l_z} z_a) \\ &\times \sin(k_{l_x} x_b) \sin(k_{l_y} y_b) \sin(k_{l_z} z_b) \\ &\times \exp \left\{ \sum_{\mathbf{q}_x = \mathbf{q}_x^{es}} R_\rho(\mathbf{q}_x) + (x \rightarrow y, z) \right\}. \end{aligned} \quad (57)$$

$$R_\rho(\mathbf{q}_x) = \frac{1}{\sqrt{N}} \left((S_1^{(1)}(\mathbf{q}_x))^* e^{-iq_x x_a} + S_1^{(1)}(\mathbf{q}_x) e^{iq_x x_b} \right). \quad (58)$$

We use approximation (28), (26). Then $S_1^{(1)}$ is real, and we can replace $e^{-iq_x x} \rightarrow \cos q_x x$ and can sum only over $q_x > 0$. We obtain

$$\rho(\mathbf{r}_a, \mathbf{r}_b) = \rho_\infty^c f_x(x_a) f_x(x_b) f_y(y_a) f_y(y_b) f_z(z_a) f_z(z_b), \quad (59)$$

$$f_x(x) = \sin(k_{l_x} x) \exp \left\{ \frac{2}{\sqrt{N}} \sum_{q_x^{es} > 0} S_1^{(1)}(\mathbf{q}_x^{es}) \cos(q_x^{es} x) \right\}. \quad (60)$$

Since $q_x^{es} = 2k_{l_x}, 4k_{l_x}, 6k_{l_x}, \dots$, we have

$$f_x(x) = \sin(k_{l_x} x) e^{\{g_2 \cos(2k_{l_x} x) + g_4 \cos(4k_{l_x} x) + \dots\}}, \quad (61)$$

where $g_j = 2S_1^{(1)}(jk_{l_x} \mathbf{i}_x) / \sqrt{N} \sim 1$. Function (61) coincides with (29), (31). Substituting (59) and (61) in (54) and expanding (61) in a series, we obtain that the condensate levels with $N_{\mathbf{k}} \sim N$ correspond to the wave

vectors $\mathbf{k} = ((1+2j_x)k_{l_x}, (1+2j_y)k_{l_y}, (1+2j_z)k_{l_z})$ with $j_x, j_y, j_z = 0, 1, 2, 3, \dots$; i.e., to the vector $\mathbf{k}_1 = \mathbf{k}_c$ and to larger vectors with odd multiple components.

The distribution of atoms over levels depends on the barrier height U_b , here we have the interesting picture. The numerical calculation for He^4 atoms with $\bar{R} = 3.6 \text{ \AA}$ and potential (33) with $a = 2 \text{ \AA}$, $b = 4 \text{ \AA}$, $U_{bd} = -9 \text{ K}$, and realistic values $500 \text{ K} \lesssim U_b \lesssim 5000 \text{ K}$ gives $g_2 \sim 1$, $g_4 \sim -0.1$, and the subsequent g_j are small. With such g_j , we obtain $N_{\mathbf{k}=\mathbf{k}_c} \approx (1 - g_2/2 + g_2^2/4)^6 \rho_\infty^c N/8$. For the higher levels, we have: $N_{\mathbf{k}=3\mathbf{k}_c} \approx (g_2/2 - g_4/2)^6 \rho_\infty^c N/8$, $N_{\mathbf{k}=5\mathbf{k}_c} \approx (g_2^2/8 + g_4/2)^6 \rho_\infty^c N/8$, $N_{\mathbf{k}=7\mathbf{k}_c} \approx (g_2 g_4/4)^6 \rho_\infty^c N/8$, etc. Hence, the levels with $\mathbf{k} = \mathbf{k}_c, 3\mathbf{k}_c$ and the intermediate ones with $\mathbf{k} = (k_{cx}, 3k_{cy}, k_{cz}), (k_{cx}, 3k_{cy}, 3k_{cz})$ (and with permutations) are filled. The rest levels are almost empty. Thus, we have 8 levels with $N_{\mathbf{k}} \sim (g_2/2)^6 \rho_\infty^c N/8 \sim \rho_\infty^c N/8^3$ atoms on each of them, in the sum $N_c \sim \rho_\infty^c N/64$. For comparison, $N_{\mathbf{k}_1} \approx \rho_\infty N/2$ for a liquid⁴³. It is easy to verify that

$$\rho_\infty^c \sim \rho_\infty^l / P^3, \quad P = \int_0^{L_x} \frac{dx}{L_x} [f_x(x)]^2. \quad (62)$$

With the obtained g_j , we have $P \simeq (1 - g_2 + g_2^2)/2 \simeq 1/2$, i.e., $\rho_\infty^c \sim 8\rho_\infty^l$. The value of ρ_∞^l is given by the formula for a fluid. Let us consider the ‘‘crystal’’ correction $A_2(\mathbf{k})$ (20) in Eq. (17) for $a_2(\mathbf{k})$. Then, for $U_b \sim 10^2\text{-}10^4 \text{ K}$, the values of $a_2(\mathbf{k})$ decrease twice (in modulus) on the average in the significant interval of k (where a_2 is not small). In the zero approximation⁴⁴, $\rho_\infty^l = \exp[-\frac{1}{N} \sum_{\mathbf{k} \neq 0} \frac{a_2^2(\mathbf{k})}{1-2a_2(\mathbf{k})}]$. We know from experiment that $\rho_\infty \approx 0.07$ for He II. At twice less $a_2(\mathbf{k})$, we obtain for He^4 atoms $\rho_\infty^l \simeq 1/3$ and $\rho_\infty^c \sim 8/3$. Hence, the condensate levels of a sc solid He^4 contain $N_c \sim 0.04N$ atoms. This is only a rough estimate.

At $U_b \gtrsim 10^4\text{-}10^5 \text{ K}$, we have $g_2 \sim 1$, g_4 takes values from -2 down to -10, $g_{j \geq 6} \approx 0$; the levels with $\mathbf{k} = 3\mathbf{k}_c, 5\mathbf{k}_c, 7\mathbf{k}_c$ and the intermediate ones are filled. At $U_b \gtrsim 10^6 \text{ K}$, the values of g_6, g_8 , and g_{10} become large, which generates the condensates with $\mathbf{k} = 9\mathbf{k}_c, 11\mathbf{k}_c, 13\mathbf{k}_c$.

As is seen, the condensate structure in a crystal is similar to that of a fluid in a vessel⁴³, but with the vector \mathbf{k}_c instead of \mathbf{k}_1 and with a different distribution over levels. Within our method, it is impossible to calculate the condensate with high accuracy, because the significant corrections were omitted in almost all equations. In this case, the Monte-Carlo method can be efficient⁴¹.

The structure of Ψ_0 (2) helps us to imagine the condensate: Ψ_0 contains N identical standing waves (the product of sines) resting on the walls by their wings. These waves form a single resonance classical wave, which modulates the motion of atoms. Therefore, many atoms are characterized by the wave vector \mathbf{k}_1 of this wave. It will be discussed in Sec. 8 that this wave can be considered as a particular kind of longitudinal sound. Therefore, the

condensate of N “zero-phonons” is present in the ground state. Thus, the resonance wave forms a crystal and supports the condensate of atoms. In a fluid, the condensate is also formed by a wave, but with $\mathbf{k} = \mathbf{k}_1$ (see I and Ref. 43).

Wave function (2) describes a simple rectangular lattice. The more complicated lattices can be constructed, by setting a relevant bare WF Ψ^{bare} instead of the product of sines Ψ_{sc}^{bare} (8). The important point is whether Ψ^{bare} reflects the structure of a Wigner-Seitz cell, i.e., whether it equals zero on its surface. This is true for the sc lattice, but is not necessarily for other lattices. If $\Psi^{bare} \neq 0$ on the cell surface (we denote $\Psi_{cell}^{bare} \neq 0$), then it is easy to guess the form of Ψ^{bare} for the bcc and fcc lattices:

$$\begin{aligned} \Psi_{bcc}^{bare} &= \Psi_{sc}^{bare}(N/2) \prod_{j=1+N/2}^N \{ \sin(k_{l_x}(x_j - a_l/2)) \\ &\times \sin(k_{l_y}(y_j - a_l/2)) \sin(k_{l_z}(z_j - a_l/2)) \} \\ &+ \text{permutations.} \end{aligned} \quad (63)$$

$$\begin{aligned} \Psi_{fcc}^{bare} &= \Psi_{sc}^{bare}(N/4) \Psi_z^{xy}(N/4) \Psi_y^{zx}(N/2) \Psi_x^{yz}(3N/4) \\ &+ \text{permutations.} \end{aligned} \quad (64)$$

$$\begin{aligned} \Psi_z^{xy}(N_0) &= \prod_{j=N_0+1}^{N_0+N/4} \left\{ \sin(\sqrt{2}k_{l_x}\hat{x}_j) \sin(\sqrt{2}k_{l_y}\hat{y}_j) \right. \\ &\times \left. \sin(k_{l_z}[z_j + a_l/2]) \right\}, \end{aligned} \quad (65)$$

$$\hat{x}_j = (x_j - a_l/2) \cos(\pi/4) + y_j \sin(\pi/4), \quad (66)$$

$$\hat{y}_j = -(x_j - a_l/2) \sin(\pi/4) + y_j \cos(\pi/4). \quad (67)$$

Here, the permutations symmetrize the WF to the Bose form, a_l is the period of a lattice, and four functions in (64) on the right-hand side depend on the coordinates of atoms with the numbers $1, \dots, N/4$; $N/4 + 1, \dots, N/2$; $N/2 + 1, \dots, 3N/4$ and $3N/4 + 1, \dots, N$. These WFs imply that, for the bcc lattice, $\mathbf{k}_c = \pi(\mathbf{i}_x + \mathbf{i}_y + \mathbf{i}_z)/a_l$, and the condensate \mathbf{k} are the same as that for the sc lattice. For the fcc lattice, there are four composite condensates: with $\mathbf{k}_c = \pi(\mathbf{i}_x + \mathbf{i}_y + \mathbf{i}_z)/a_l$ and $\mathbf{k}'_c = \pi(\sqrt{2}\mathbf{i}_x + \sqrt{2}\mathbf{i}_y + \mathbf{i}_z)/a_l$ with permutations of x, y, z .

At $\Psi_{cell}^{bare} = 0$, \mathbf{k}_c are different. For the sc lattice, the basis vectors of the reciprocal lattice are $\mathbf{b}_1 = 2\pi\mathbf{i}_x/a_l$, $\mathbf{b}_2 = 2\pi\mathbf{i}_y/a_l$, and $\mathbf{b}_3 = 2\pi\mathbf{i}_z/a_l$, and the relation $\mathbf{k}_c = \mathbf{g}_0^{3D}/2 \equiv (\mathbf{b}_1 + \mathbf{b}_2 + \mathbf{b}_3)/2$ holds. For the bcc lattice, we have $\mathbf{b}_1 = 2\pi(\mathbf{i}_y + \mathbf{i}_z)/a_l$, $\mathbf{b}_2 = 2\pi(\mathbf{i}_x + \mathbf{i}_z)/a_l$, and $\mathbf{b}_3 = 2\pi(\mathbf{i}_x + \mathbf{i}_y)/a_l$, and the relation $\mathbf{k}_c = \mathbf{g}_0^{3D}/2 = 2\pi(\mathbf{i}_x + \mathbf{i}_y + \mathbf{i}_z)/a_l$.

We note that the solution for a one-particle WF with spherical orbit was studied in Ref. 25. There, it was assumed that the atoms of the condensate have $k \sim 2.1 \text{ \AA}^{-1}$. This is close to our results.

It is of importance to confirm the existence of the condensate in experiments. A neutron or a photon are scattered with the creation of a quasiparticle or elastically. In the second case, the wave vector of the scattering atom either is not changed or changes only the direction (to the opposite one), and the state of the crystal is invariable (except for the recoil). If the condensate is present, then the scattering with the momentum transference $2\mathbf{k}_c$ (or with a change in one-two components of the vector $2\mathbf{k}_c$) gives the intense peak. At $\Psi_{cell}^{bare} = 0$ and at $\Psi_{cell}^{bare} \neq 0$, these changes in the momentum are equal to the vector \mathbf{g} of the reciprocal lattice, and the scattering corresponds to the Bragg-Wolf (BW) peaks. But if $\Psi_{cell}^{bare} = 0$, then the number of condensate peaks is less than that of BW peaks. At $\Psi_{cell}^{bare} \neq 0$, the intensity of all BW peaks must increase at small T (in the presence of a condensate) proportionally to the amount of the condensate. For bare WFs (8), (63)–(65), the BW peaks (noncondensate ones) can be, apparently, interpreted as a result of the scattering by zero-phonons with $\mathbf{k} = \mathbf{k}_c$.

For the bcc, fcc, and hcp lattices, the Wigner-Seitz cell is complicated. Moreover, at $\Psi_{cell}^{bare} = 0$, its creation requires a wave with complicated structure. But, at $\Psi_{cell}^{bare} \neq 0$, the lattice can be formed from waves with a simpler structure of the type (63)–(66). Since the Nature uses simple structures, we suppose that $\Psi_{cell}^{bare} \neq 0$.

We note that $\mathbf{k} = \mathbf{k}_c + \delta\mathbf{k}$ for the higher condensates, and the components $\delta\mathbf{k}$ are multiple to the components $2\mathbf{k}_c$. Therefore, all condensates must be revealed in experiments as a part of the “base” condensate with $\mathbf{k} = \mathbf{k}_c$.

V. COMPARISON WITH THE TRADITIONAL APPROACH

Let us compare the wave solution (2) with the traditional one (1). In the last case, it is assumed that the atoms carry on small oscillations near lattice points.

The traditional approach involves several assumptions. 1) The lattice is set “by hands”, it is not obtained from the Schrödinger equation. 2) It is assumed that the probability density maximum in a cell is located at the lattice point, near which the atom carries on random oscillations (atom is fixed likewise on rubber string, which role is played by the function $\varphi(\mathbf{r} - \mathbf{R})$). Here, one more courageous assumption is hidden: that the mechanism of appearance of a lattice does not influence the motion of atoms in it. 3) It is assumed also that the boundaries have no effect on the solutions. Therefore, the realistic BCs close to zero ones are replaced by the cyclic conditions.

Solution (2) has no above-mentioned drawbacks. It is found with the use of natural zero BCs. The lattice and the probability distribution in a cell do not postulated, but they follow from the solution of the Schrödinger equation. It is seen from the probability distribution that the motion of atoms is strongly affected by the mechanism (wave one) of formation of a crystal. In addition, the

observable quantities, in particular E_0 and the energy of phonons, depend significantly on the BCs. This is caused by the fact that the walls change the Fourier expansion of the two-particle potential (see I: formulas (15)-(17) and Sec. 5) and affect the phonon frequency through Ψ_0 . Visually, it is because the excitations of the quantum system are standing waves rather than particles; a wave keeps the memory about the wall and its length is modulated by the wall. Such influence exists only for natural long-range potentials. In the above equations for E_0 and $E(k)$, this influence is manifested in the factor $1/8$ at the potential $\nu_3(k)$ and in the summation over the wave vectors multiple to π/L , rather than $2\pi/L$, in a corrections. To the effect of boundaries, we can refer also the corrections Q_j (changing the phonon frequency $E(k)/\hbar$), which arise from the product of sines in (2) and are induced by the interaction of a phonon with N zero-phonons of the ground state.

Relation (2) yields easily the traditional solution (1). Let each atom be localized near a lattice point, one atom per point. The points \mathbf{R}_j correspond to the extrema of a sine. By expanding the sines in a Fourier series near points, the terms linear in $\mathbf{r}_j - \mathbf{R}_j$ are absent, and the small quadratic terms can be taken up in the exponent. Thus, for the sc lattice, we have

$$\begin{aligned} & \prod_{j=1}^N \{ \sin(k_{l_x} x_j) \sin(k_{l_y} y_j) \sin(k_{l_z} z_j) \} \\ & \rightarrow \pm \prod_{j=1}^N e^{-\alpha^2 (\mathbf{r}_j - \mathbf{R}_j)^2 / 2}, \end{aligned} \quad (68)$$

where $\alpha = k_{l_x} = \pi/\bar{R}$ (the close estimate $\alpha \simeq 1 - 2 \text{\AA}^{-1}$ was obtained in Ref. 1 from the other reasoning). By setting $S_w^{(1)} = 0$ in (2), we reduce (2) to (1).

Thus, the traditional solution (1) is a simplification of the wave solution (2). It is significant that, in this case, the wave character of the solution is lost; but since the counting-off is made from the equilibrium positions of atoms, it is sufficiently simple to calculate^{1,29-32,35,38,39} (with several fitting parameters) E_0 and $E(k)$. In this respect, approach (1) has certain advantages, since the wave approach (2) yields a chain of complicated equations with many large corrections for E_0 and $E(k)$. These equations cannot be solved exactly.

The frequency of phonons $E(k)/\hbar$ is usually calculated in the harmonic approximation, where a phonon is a wave arising at a small deviation of atoms from equilibrium positions. However, it was noted above that the phonon frequency is affected by zero-phonons. In the language of oscillating atoms, this means that the atoms in the ground state are not in rest at lattice points (as is considered in the harmonic approximation), but they oscillate intensively due to the motion in the field of zero-phonons. In this case, the potential energy is minimum, probably, at lattice points. But it would be wrong to identify the deviations from “equilibrium positions” with the coordinates of real atoms, since, in this case, the intense

zero oscillations would be lost. Therefore, the harmonic approximation is applicable only for the description of long-wave oscillations, when a crystal can be considered as a continuum. This approximation cannot be used for short-wave phonons, and the corresponding approaches in solid-state physics should be reconsidered, in our opinion. The agreement with experiment of phonon dispersion curves calculated in the harmonic approximation in a number of works seems to be accident or is due to the choice of parameters.

WF (1) is not a solution of the Schrödinger equation. The attempt to determine $\varphi(\mathbf{r} - \mathbf{R})$ in (1) from the Schrödinger equation leads¹ to the solution $\varphi(\mathbf{r} - \mathbf{R}) \sim e^{i\mathbf{k}\mathbf{r}}$, which is nonlocalized and, therefore, unphysical. It was assumed¹ that this liquid-like solution arises due to the truncation of the cluster expansion. However, instead of $e^{i\mathbf{k}\mathbf{r}}$, we can take a linear combination of exponents $\varphi(\mathbf{r} - \mathbf{R}) \sim \sin(k_{l_x} x) \sin(k_{l_y} y) \sin(k_{l_z} z)$. Then we arrive at the wave solution (2), which is quite physical and sets a lattice with localized distribution of atoms.

Recently, N. Prokof'ev³ considered a wave solution of the form

$$\Psi = \prod_{i=1}^N \left(\frac{1}{\sqrt{N_L}} \sum_{j=1}^{N_L} \varphi(\mathbf{R}_j - \mathbf{r}_i) \right), \quad (69)$$

which contains a condensate in the state $\frac{1}{\sqrt{N_L}} \sum_{j=1}^{N_L} \varphi(\mathbf{R}_j - \mathbf{r})$. However, this solution was recognized unphysical³, because the number N_L of the lattice points can differ from the number N of atoms. Hence, the solution for a crystal is only one of the huge number of solutions, and the probability of its realization is too small. We note that N_L in (2) can also be different from N . However, it is easy to see (see the following section) that we have no problems in this case.

Thus, solution (2) can be obtained long ago.

In the last time, the following new approaches to the description of quantum crystals are developed: Path Integral Monte-Carlo method⁴¹, variational Shadow WFs method⁴⁵ using the bare WF (1) and many fitting parameters, and Shadow Path Integral Ground State projector method²⁰. The last method used the Bijl-Jastrow function, and the lattice arises due to the spontaneous breaking of symmetry.

VI. GROUND STATE — LIQUID OR CRYSTAL?

It is accepted that most substances in the ground state are crystals. Apparently, the ground state corresponds always to a liquid.

The question about the structure of the ground state can be answered, by seeking a minimum of the energy. Consider a sc crystal. Its ground-state energy is given by formula (36). In (36), we fix the number of atoms N (i.e., the value of \bar{R}) and change the number of points N_L

(i.e., the value of k_c). In the zero approximation (32) for $a_2(k)$, the curve $E_0(k_c)$ is a parabola (see Fig. 4), where the point $k_c \approx 1.41 \text{ \AA}^{-1}$ corresponds to $N_L = N$. If we descend somewhat downward along the curve, we obtain the states with $N_L < N$, where some cells have two atoms. In such cells, the distance between two atoms must be small, $\simeq \text{\AA}$. Since the atoms have the almost hard core with a radius of $1.2 - 1.3 \text{ \AA}$, they strongly repel each other at distances of $\lesssim 2.5 \text{ \AA}$. Therefore, such solution is unstable: one of the atoms leaves the cell and will walk in the crystal, until it approaches the crystal surface. There, the atom evaporates or becomes fixed. As a result, the system transits in the state with $N_L = N$. If we lift upward along the curve, we obtain the states with vacancies ($N_L > N$). Such states have higher energies. Hence, the stable state of the crystal with minimum energy has $N_L = N$, and each cell contains exactly one atom. This reasoning answers the objection in Ref. 3.

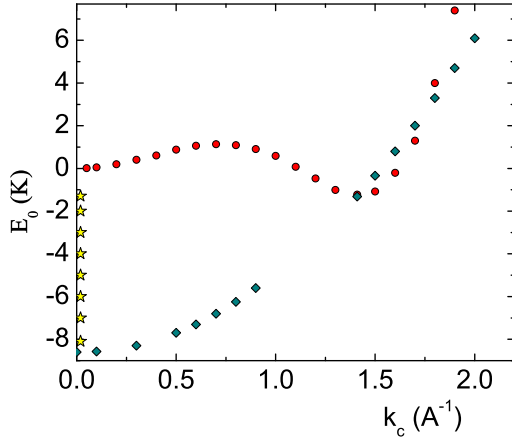


Fig. 4: Function $E_0(k_c)$ for a sc lattice of He^4 atoms at the fixed $\bar{R} = 3.85 \text{ \AA}$ (rhombs) and the variable \bar{R} under the condition $N_L = N$ (circles). Stars show the underliquid at various temperatures. We use the potential (33) with $a = 2 \text{ \AA}$, $b = 4 \text{ \AA}$, $U_{bd} = -9 \text{ K}$ and $U_b = 81.2 \text{ K}$.

The curve of rhombs indicates that $E_0(k_c = 1.6 \text{ \AA}^{-1}) \approx E_0(k_c = 1.41 \text{ \AA}^{-1}) + 1.1 \text{ K}$. At $k_c \approx 1.6 \text{ \AA}^{-1}$, the system has 0.46 vacancy per atom. Hence, the vacancy energy $E_v \approx 2.4 \text{ K}$, which is comparable, by the order of magnitude, with experimental value⁴⁶ $E_v \sim 10 \text{ K}$.

The dependence $E_0(N)$ (circles in Fig. 4) is quite reasonable: the most favorable state of the lattice corresponds to the minimum ($k_c \approx 1.41 \text{ \AA}^{-1}$, $\bar{R} \approx 3.85 \text{ \AA}$). By passing to a rarefied system ($\bar{R} \rightarrow \infty$, $k_c \rightarrow 0$), we have $E_0 \rightarrow 0$.

The minimum of the parabola of rhombs corresponds to the least possible $k_c = k_1 = \sqrt{3}\pi/L$, at which WF (2) transits in Ψ_0 of a fluid, and E_0 (36) is determined only by the term \bar{E}_0^b for fluids. Hence, the ground state of a fluid ($E_0 \approx -8.6 \text{ K}$) lies below the ground state of the crystal ($E_0 \approx -1.27 \text{ K}$). The states on the parabola near

the minimum (e.g., with $k_c \sim 0.1 \text{ \AA}^{-1}$) correspond to a fluid partitioned into domains with many atoms. Such states must be unstable.

We have studied Eq. (36) obtained in a rather crude approximation. Its solution can be changed with regard for corrections and the exact potential (with a higher barrier). It can turn out that the ground state includes the admixture of vacancies¹⁷, though this is improbable.

The main question is as follows: *Is E_0 of a crystal greater than E_0 of a liquid or less, for the exact solution?* The answer is hinted by the node theorem⁴⁷: “if the eigenfunctions of a self-adjoint second-order differential equation are arranged in some region G under any homogeneous BCs in the increasing order of the appropriate eigenvalues, then the nodal manifolds of the n -th eigenfunction Ψ_n divide the region G into at most n subregions for any number of independent variables”. The theorem was proved for WFs of the general form $\Psi(\mathbf{r}_1, \dots, \mathbf{r}_N)$. We deal with the WFs of N identical Bose particles, and the conditions of the theorem are satisfied. We know that WF (2) with $\mathbf{k}_1 \rightarrow \mathbf{k}_1$ corresponds to the ground state of a liquid and has no nodes. By the theorem, namely this function describes the ground state of a system of Bose particles in a box. Hence, all remaining states, including the ground state of the crystal, have nodes and correspond to higher energies. But it can be so that the equations have no solutions for Ψ_0 corresponding to a liquid. Does Ψ_0 of the crystal without nodes exist? It is clear that, at the wave structure of (2), the WF of the crystal has necessarily nodes. Can a nonwave structure be realized? The WF must turn to zero at the surface of the crystal and be symmetric under permutations of atoms. It is easy to see that the nonwave solution (1) is impossible without nodes: it does not feel the boundaries and can become zero only at infinity. We cannot strictly prove this assertion, but we sure that only the wave solution satisfies the zero BCs. This implies that 1) the ground-state energy of the crystal is always higher than that of a liquid composed of the same atoms; 2) the solution for Ψ_0 describing a liquid exists necessarily for Bose atoms of all sorts (if the solution is absent at some density ρ of a liquid, it is possible to enter a region, where a solution exists, by varying ρ).

However, the majority of substances in the Nature become crystals at low temperatures. The transition in the crystal state allows the system to decrease the energy by jump and is favorable. But it is seen in Fig. 4 that the principal minimum corresponds to a liquid. Apparently, by “having fallen” in the crystal state, the system cannot already pass to a deeper minimum corresponding to a liquid. To make this, the system must overcome a band of unstable state (or the energy barrier that can appear at the exact solution). Therefore, the majority of substances at low temperatures are crystals.

The state of a liquid in the deep minimum can be called the underliquid (UL, stars in Fig. 4). Most probably, the majority of ULs has the superfluid phase. The temperature (determined by quasiparticles) of UL can be equal to

the temperature of a crystal, but the total energy is less than that of the crystal. He^4 atoms have a large amplitude of zero oscillations. Therefore, the lattice is locally unstable, apparently, and transits in the UL state. In other words, He II is the single example of UL among inert elements. Possibly, other substances can be also transferred in the UL state (see Sec. 8). The amorphous bodies with microstructure of a liquid are not related, apparently, to UL, since the amorphous state is caused by a strong anisotropy of molecules, whereas we have considered the systems of spherical molecules.

We arrive at a significant conclusion that a finite system of Bose particles of any sort (He, Ar, Ne, etc.) in the lowest state is a liquid, rather than a crystal, as is commonly accepted. Sometimes, the third law of thermodynamics and the entropy-based arguments in favor of a crystal are discussed. However, the entropies of a crystal and a liquid in the ground state are identical and are equal to zero: $S = k_B \ln N_s = k_B \ln 1 = 0$. In other words, the degrees of order of a fluid and a crystal are identical in the ground state, though a crystal seems visually to be more ordered.

VII. NATURE OF THE SUPERSOLID PHASE

Almost all researchers arrived at the consensus^{3,20–22,26,41,48} of that the supersolid phase and NCIM^{4,5} are related to defects of the lattice. However, the attempts to identify a carrier of NCIM with a specific defect met difficulties, which is not surprising. How can a crystal contain so many defects (or so extended defects) at ultralow temperatures $T \simeq 0.02$ K that they connect 20% of atoms of the lattice, by ensuring the experimental value $\rho_s \simeq 0.2\rho$? In our opinion, it is improbable. We note that the defects are an analog of quasiparticles; for comparison: the amount of quasiparticles in He II at $T = 0.02$ K is so small that they provide $\rho_n \sim 10^{-7}\rho$. Therefore, we suppose that the carriers of the effect are atoms of the ideal lattice.

Let us consider various possibilities in detail. We start from vacancies. Since any crystal is in the gravity field, the vacancies undergo the action of the force directed upward. If the gas of vacancies is superfluid, then the vacancies should float up rapidly and evaporate from the surface. Under torsional oscillations, they must be transported to an internal surface of a crystal. Since this reasoning is valid for any massive defects, NCIM is not related to vacancies.

The models of dislocation glass²³, superglass²¹, and grain boundaries²² assume the existence of the condensate of atoms with $k = 0$, but it was not observed⁴²: $n_0 \lesssim 0.003$. In the model of screw dislocation network²⁴, the superfluid component consists of atoms of the nuclei of dislocations, whose amount is obviously much less than 10%. Therefore, this model does not explain the observed large values of $\rho_s \simeq (0.1 - 0.2)\rho$. The models of dislocation network met the analogous difficulty^{18,23}. As for

the mechanism of grain boundaries²², it does not agree with the fact that NCIM was observed in a monocrystal¹⁰ (where any grains are absent).

As carriers can be atoms of the lattice. It was proposed already²⁵, but no mechanism of correlations (of the condensate) was indicated. We propose the following scenario. For the sc lattice, $\Psi_0 = 0$ on the boundary of a Wigner-Seitz cell. Therefore, the atom cannot pass from a cell to another one. However, for the bcc, fcc, and hcp lattices, $\Psi_0 \neq 0$ most probably on the boundary of a cell (see Sec. 4), and the tunneling of an atom from cell to cell is possible. Consider a bcc crystal. According to Sec. 2, the atom is located near the orbit, whose size is twice less than that of a cell of the crystal. The orbits of the atom at the center of a cubic cell and the atom of one of eight vertices of a cube touch each other. Therefore, the WFs of such atoms are strongly overlapped. If the condensate includes more than a quarter of atoms, then each atom is contiguous to two or more atoms of the condensate. In this case, many neighboring atoms of the condensate can be joined by lines. Along such closed lines, the atoms can flow by means of the simultaneous tunneling (according to the structure of WF (63), one atom cannot flow through a crystal, since the zeros of a sine create the impermeable planes in a certain distance). Due to the indistinguishability of atoms, the atoms belonging to the condensate and the overcondensate change places. Therefore, all atoms participate in the flow. Since the atoms of the condensate are correlated, they can move as the whole, by representing the flowing component of a crystal. In order that this component be superfluid, its excitations must satisfy the Landau criterion. The dispersion curve of such excitations was apparently observed^{13,14}, and it satisfies the Landau criterion. We assume that the superfluidity is possible only in the case where the concentration n_c of the condensate is higher than the threshold one ($n_c^{cr} = n/4$ for the bcc lattice). Sec. 4 indicates that such n_c is possible.

Let us turn to the optic-like dispersion curves^{13,14}. They are very close, and we can have no doubts that they represent the same mode. In Ref. 13, this mode was considered vacancional. But the experiment¹⁴ with a polycrystal showed that it disappears at $0.2 \text{ K} < T < 0.6 \text{ K}$. Though, the ordinary vacancional mode must be present at all T ; it shifts only, as the density varies⁴⁶. In Ref. 14, the mode is referred to the superfluid component, and we agree with it. However, it is the mode related to a crystal (rather than to a liquid¹⁴), because the minimum is just at the Brillouin zone boundary. According to our approach, this superfluid mode must appear at the cooling of a crystal down to the temperature, where the tunneling of the condensate starts. It is T_{NCIM} , the temperature, where the effect of NCIM arises. This is in agreement with data¹⁴. In Ref. 13, the mode was observed also at $T = 0.6 \text{ K}$, which is more than the known T_{NCIM} . But, in that case, a monocrystal was used. For it, T_{NCIM} is unknown and can exceed 0.6 K. We mention one more optic-like mode⁴⁹ observed for the bcc lattice of He^4 . It

should be noted that the data in Refs. 13,14,49 say nothing about the nature of the superfluid component, which can be vacacional.

We note that since the flow can occur only through lattice points, and some condensate chains can break, the atoms of the condensate must be involved in torsional oscillations of a crystal only partially. So that NCIM is proportional to qn_c , where $q < 1$. The value of q is decreased by various defects. Therefore, q must strongly depend on the conditions of an experiment (this is observed), and ρ_s can be small at high n_c . The maximum of q for the crystals with a large ratio of area to volume¹² can be explained by the disappearance of large defects hampering the flow of the condensate. It is clear that the effect is maximum for the ideal crystal without admixtures and defects.

We note that the destruction temperature for the condensate must be significantly higher than T_{NCIM} , since the tunneling flow requires $n_c \geq n_c^{cr}$.

The proposed tunneling mechanism agrees with the absence of the superfluidity of crystals at a pressure gradient^{7,8}. According to Refs. 7,8, the superfluidity should be accompanied by a deformation of the lattice (if defects are absent). But, at the tunneling mechanism, the atoms can move in the lattice without any change of its shape. Namely the torsional oscillations^{4,5} present the conditions for such motion. At the tunneling mechanism, the crystal cannot also shift as a whole, since, to realize it, the surface atoms must tunnel outside of the crystal, where there are no lattice points. For the same reason, one more possible mechanism⁸ such as the leakage of atoms of a fluid through a crystal is forbidden. All this corresponds to the conclusion⁷ that the mechanisms of flows for a crystal and a fluid are quite different.

A decrease of NCIM after the annealing⁶ can be related not to a decrease in the number of defects, but to the appearance of lengthy defects. It is well known that a bullet piercing glass makes only a small hole, whereas a stone creates additionally a network of long cracks. In other words, the slow processes are accompanied by extended deformations of a crystal. Under the annealing, a crystal is firstly strongly heated and then is slowly cooled. In this case, the majority of defects disappear, but the remaining dislocations are ordered into a three-dimensional network⁵¹, which hampers the flow of the condensate to a higher degree than many disordered dislocations.

The effect of NCIM was mainly observed in polycrystals. The tunneling of atoms in them is possible, since there are no slits between microcrystals.

The experimentally found¹¹ law $\Delta p \sim T^2$ (it is equivalent to $C_v \sim T$) can be because the condensate density is close to the threshold value: $n_c \simeq n_c^{cr}$. In this case, the dimension of the network of lines, by which the condensate flows, is close to 1.

The jump of the rigidity of a crystal^{9,16} at $T \approx T_{NCIM}$ means that the same factor affects the rigidity and NCIM. We assume that this factor is the appearance of the superfluid component. As a result, a part of energy

is transferred to modes of the superfluid component, and there occurs a redistribution of oscillatory modes of the system. This causes the jump of the rigidity. An increase of NCIM⁵⁰ due to He^3 atoms can be related to the fact that He^3 atoms join dislocations and, under the action of the inertial force at torsional oscillations, turn a dislocation or move it to the surface of a crystal.

It is necessary to understand why the heat capacity peak is less for purer crystals, and the temperature T_{C_v} of the peak is less than T_{NCIM} and is independent of the concentration of the He^3 admixture¹⁵ (though T_{NCIM} depends strongly on it). The first property is similar to the annealing effect. We assume that the reason is the same: purer (on the average) crystals contain more lengthy defects. Consider now the second and third properties. The “excess” of C_v is related to the superfluid subsystem and increases approximately linearly¹⁵ at low T . As T increases, a part of chains, on which the superfluid flow is realized, is broken due to the approach of n_c to the threshold and the freezing-out of defects. Let a half of chains be broken. If many alternative chains remain, then NCIM is almost not changed, but the number of modes of the superfluid subsystem (i.e., C_v also) decreases twice. NCIM decreases sharply only if the number of chains becomes so little that the atoms lose the ability to flow. Apparently, as T decreases, the superfluidity arises gradually: first, a small number of atoms of the condensate can flow. In this case, NCIM and the peak of C_v are not related to the phase transition, $T_{NCIM} > T_{C_v}$, and the peak of C_v is independent of the He^3 admixture and is caused by the dependence of the number of phonons in the condensate network of atoms on the properties of this network.

As is seen, the proposed model can explain the super-solid phenomenon, but remains many questions unsolved. It should be clarified whether Ψ_0 becomes zero on the surface of a Wigner-Seitz cell for the bcc and hcp lattices. It is also necessary to know which and how many defects are present in a crystal under various conditions, and how each sort of defects influences the condensate and its fluidity. The key moment for the model is the experimental discovery of a composite condensate with $\mathbf{k} = \mathbf{k}_c, 3\mathbf{k}_c, 5\mathbf{k}_c$.

VIII. DISCUSSIONS

It is seen from formula (2) that a crystal is formed by a standing wave in the probability field. A fluid has an analogous wave, but with $\mathbf{k} = \mathbf{k}_1 = (\pi/L_x, \pi/L_y, \pi/L_z)$. In I, it is shown that the wave in a fluid is similar to N standing sound waves with $\mathbf{k} = \mathbf{k}_1$. The same arguments are true also for a crystal. Therefore, we can assert that a crystal in the ground state has N identical standing longitudinal acoustic phonons with $\mathbf{k} = \mathbf{k}_c$. They are particular resonance zero-phonons. By the structure of corrections, they differ from ordinary phonons described by WF (37)–(40). It is significant that these standing

zero-phonons create a crystal lattice. In other words, the *periodicity of a crystal is caused by the periodicity of a sound wave*.

The number of resonance phonons is equal to the number of atoms. At such huge occupation number, these phonons can be considered as a single classical sound wave. But if a crystal is a wave, we can try to control its state with the help of sound and electromagnetic waves. In particular, it would be possible to create or to destroy crystals.

Well-known are the legends concerning N. Tesla⁵², who induced vibrations of building's walls with the help of a small mechanical oscillator with the resonance frequency in the ultrasound region. Apparently, N. Tesla excited the eigenmodes with \mathbf{k} (5). The particular resonance frequency for crystals is the frequency of zero-phonons, which is equal to the difference of E_0/\hbar of a crystal and E_0/\hbar of a fluid. The wave with such a frequency forms a crystal itself.

In Sec. 6, the state of underliquid is predicted. Possibly, this state can be obtained by means of the wave action on a crystal or a rapidly cooled fluid (so that the fluid will avoid the state of crystal and become UL). Through a liquid, it is necessary to transmit monochromatic sound or electromagnetic waves with a wavelength comparable (but not equal to) with the period of a lattice. It is possible to use an x-ray or gamma-laser with $0.5 \text{ \AA} \lesssim \lambda \lesssim 10 \text{ \AA}$. But such lasers have not been created till now, to our knowledge. A crystal can be destroyed, possibly, by a wave with the frequency of a zero-phonon. All this remains else at the level of speculations, but it is interesting to study these questions.

The crystallization of a liquid can be related to resonance phenomena in the system of phonons. The centers of crystallization are usually considered in the language of interacting atoms. But, according to the wave solution, these centers are, most likely, growing wave packets with $\mathbf{k} = \mathbf{k}_c$.

We assume that the wave principle is the general one for the formation of crystals. As an important task, we indicate the search for the solutions for the bcc, fcc, and hcp lattices, which are most spread in the Nature.

IX. CONCLUSIONS

Our most important conclusion concerns the wave nature of Bose crystals. The wave properties yield the condensate of atoms and the possible superfluidity of a crystal. If the crystals in the Nature are created by standing waves, it is quite beautiful.

The complexity of properties of quantum crystals is related to the fact that they have five subsystems: atoms of the lattice, atoms of the condensate, quasiparticles in both these systems, and various defects. This makes it difficult clarifying the nature of the supersolid phase. Though He II has only two subsystems, the superfluid subsystem and that of quasiparticles, the nature of its superfluidity was understood in more than one decade.

The properties of quantum crystals are fine and arouse the feeling of admiration. In addition, it seems clearly that Lady Science moves away from Truth sometimes in her walks. But She goes not so quickly, as the Universe expands, and can return always.

The present work is devoted to the memory of Petr Ivanovich Fomin.

X. APPENDIX. CALCULATION OF $C_l(j)$

Formula (12) arises from the expansion of $\tilde{f}(x)$ (11) in a Fourier series as $\delta \rightarrow 0$. Instead of $\tilde{f}(x)$, we can take any function, which satisfies the conditions for the Fourier expansion to exist and passes to $\cot(k_{l_x}x)$ as $\delta \rightarrow 0$. Since the input function can be expanded in a Fourier series at $\delta \neq 0$, the quantity $C_{l_x}(j_x)$ can be determined by the formulas of Fourier analysis:

$$\begin{aligned} C_{l_x}(j_x) &= -C_{l_x}(-j_x) = \lim_{\delta \rightarrow 0} \frac{1}{L_x} \int_0^{L_x} dx \tilde{f}(x) e^{-i2\pi j_x x / L_x} \\ &= \frac{1}{L_x} \int_0^{L_x} dx \cot(k_{l_x}x) e^{-i2\pi j_x x / L_x} \\ &= -2i \int_0^{1/2} dx \sin(2\pi j_x x) \cot(\pi l_x x). \end{aligned} \quad (70)$$

Integral (70) is defined, despite the discontinuities of a cotangent, and can be calculated in the sense of the principal value of an improper integral⁵³. By induction, relation (70) yields $C_{l_x}(j_x) = -i$ at $j_x = l_x, 2l_x, \dots$, and $C_{l_x} = i$ at $j_x = -l_x, -2l_x, \dots$. However, the proof of the third part of (13), namely the vanishing of C_{l_x} at the rest j_x , is not a simple task.

We use the following trick. In I, it was shown that

$$\cot(\pi x / L) = -i \sum_{j \neq 0} (j/|j|) e^{i2\pi j x / L}. \quad (71)$$

This equality should be understood in the same meaning as (12), which was obtained in I from the Fourier expansion of the smooth function $\cot(k_{1x}x + \delta_{1x})$ as $\delta_{1x} \rightarrow 0$. Formula (71) follows also from the sum of two geometric progressions:

$$\begin{aligned} \cot(\pi x / L) &= \left\{ -i \sum_{j=1,2,\dots} e^{j(-\delta+i)2\pi x / L} \right. \\ &\quad \left. + i \sum_{j=-1,-2,\dots} e^{j(\delta+i)2\pi x / L} \right\} \Bigg|_{\delta \rightarrow 0}, \end{aligned} \quad (72)$$

where $\delta > 0$, $x \in [0, L]$. Replacing $x \rightarrow l_x x$ in (71) or (72), we obtain (13).

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